STRUCTURES OF SUBSTRATE BINDING POCKETS OF SCF COMPLEXES

FIELD OF THE INVENTION

The present invention relates to binding pockets of Skp1-Cdc53/Cullin-F-box protein (SCF) E3 ubiquitin ligases associated with substrate selection and/or orientation. In particular, the invention relates to a crystal comprising such binding pockets. The crystal may be useful for modeling and/or synthesizing mimetics of a binding pocket or ligands that associate with the binding pocket. Such mimetics or ligands may be capable of acting as modulators of the interactions of an SCF E3 ubiquitin ligase and its substrates, and they may be useful for treating, inhibiting, or preventing diseases modulated by such interactions.

Methods are also provided for regulating an SCF E3 ubiquitin ligase comprising changing a binding pocket associated with substrate selection and/or orientation.

BACKGROUND

The ubiquitin proteolytic system controls the precisely timed degradation of regulatory proteins in signaling, development and cell cycle progression. Substrate ubiquitination is catalyzed by a cascade of enzymes, termed E1, E2 and E3, which activate and then conjugate ubiquitin to the substrate (Hershko and Ciechanover, 1998). E3 enzymes, also known as ubiquitin ligases, contain substrate-specific recognition domains and catalyze the final step in ubiquitin transfer. Recognition is mediated by primary sequence elements in the substrate, referred to as degrons (Varshavsky, 1991). Control of the E3-substrate interaction forms the basis for regulated proteolysis; often post-translational substrate modification, most commonly phosphorylation, serves to target substrates to their cognate E3 enzymes (Deshaies, 1999). Two main classes of E3 enzyme are now evident, as characterized by the presence of either a HECT domain or a RING domain. The HECT domain class forms a catalytically essential thioester with ubiquitin, whereas the RING domain class relies on the E2 enzymes to provide catalytic activity (Pickart, 2001). The RING domain forms an E2 docking site and orients the substrate with respect to the E2.

Phosphorylation-dependent degrons direct substrates to a recently described class of multisubunit E3 enzymes termed Skp1-Cdc53/Cullin-F-box protein (SCF) complexes. SCF complexes are built on an invariant core machinery comprised of the adapter protein Skp1, the scaffold protein Cdc53 (called Cul1 in metazoans), and the RING-H2 domain protein Rbx1 (also called Roc1 or Hrt1), which interacts with an E2 enzyme, usually Cdc34 (Pickart, 2001). Substrates are brought to the core complex by one of a large family of variable adapter subunits called F-box proteins, each of which targets a limited number of specific substrates (Bai et al., 1996, Patton et al., 1998). F-box proteins typically have a bipartite structure with an N-terminal ~40 amino acid F-box motif and a C-terminal protein-protein interaction domain, such as WD40 repeats or leucine rich repeats, which bind substrates (Bai et al, 1996; Feldman et al, 1997; Skowyra et al., 1997). The overall architecture of SCF complexes is conserved in several

related ubiquitin ligase complexes including the Anaphase Promoting Complex/Cyclosome and the Von Hippel Lindau (VHL) tumor suppressor protein complex, each of which contain cullin family members, RING-H2 domain and substrate recognition subunits (Pickart, 2001; Kaelin, 2002).

Cell cycle progression depends on the precisely timed elimination of cyclins and cyclin-dependent kinase (CDK) inhibitors by the ubiquitin system (Harper et al, 2002). In yeast, G1 cyclin CDK activity phosphorylates a CDK inhibitor called Sic1, whose degradation is necessary for onset of B-type cyclin CDK activity and DNA replication (Schwob et al., 1994). Phospho-Sic1 is specifically recognized by the F-box protein Cdc4, which recruits Sic1 for ubiquitination by the Cdc34-SCF complex (Bai et al., 1996; Feldman et al., 1997; Skowyra et al., 1997). Stable forms of Sic1 that lack CDK phosphorylation sites cause a G1 phase arrest (Verma et al., 1997), whereas deletion of *SIC1* causes premature DNA replication and rampant genome instability (Lengronne and Schwob, 2002). Cdc4 recruits several other substrates to the SCF core complex in a phosphorylation dependent manner, including the Cln-Cdc28 inhibitor/cytoskeletal scaffold protein Far1, the replication protein Cdc6 and the transcription factor Gcn4 (Patton et al., 1998). The F-box protein Grr1 functions in an analogous manner to render G1 cyclins unstable throughout the cell cycle, in a manner that depends on recognition of phospho-epitopes by the LRR domain of Grr1 (Skowyra et al, 1997; Hsiung et al, 2001).

In the metazoan cell cycle, SCF complexes target phosphorylated forms of the CDK inhibitor $p27^{Kip1}$ and cyclin E, among other substrates. Interestingly, F-box protein specificity for these substrates is reversed compared to yeast, in that the WD40 domain of hCdc4/Fbw7/Ago/SEL-10 recognizes cyclin E (Strohmaier et al., 2001; Koepp et al., 2001; Moberg et al., 2001), whereas the LRR domain of Skp2 recognizes $p27^{Kip1}$ in conjunction with the CDK-binding protein Cks1 (Harper, 2001). Both of these degradation pathways are perturbed in cancer cells. Many primary tumors express high levels of Skp2, which leads to premature degradation of $p27^{Kip1}$ and cell cycle entry (Harper, 2001). Conversely, loss of Cdc4 function causes deregulation of cyclin E-CDK2 activity, which leads to precocious S phase entry and genome instability (Spruck et al., 1999). Mutations in the *Drosophila* homolog of *CDC4*, called *ago*, were isolated as homozygous recessive alleles in a screen for excess cell proliferation, a defect attributed to ectopic cyclin E activity (Moberg et al., 2001). Mutations in *hCDC4* have been detected in several cancer cell lines that exhibit high levels of cyclin E (Moberg et al., 2001; Strohmaier et al., 2001), as well as in a significant fraction of primary endometrial cancers (Spruck et al., 2002). In addition, *hCDC4* is located in the 4q32region, which is often deleted in various cancers (Spruck et al., 2002). Significantly, a high level of cyclin E correlates strongly with low survival rates in breast cancer (Keyomarsi et al., 2002). Other important substrates appear to be targeted for degradation by Cdc4 orthologs in a phosphorylation-dependent manner, including actived forms of the developmental regulator Notch and the presenilins, which are implicated in familial early onset Alzheimer's disease (Lai, 2002; Selkoe, 2001). SCF-dependent proteolysis also mediates other important signaling events, including phosphorylation-dependent degradation of the NFκB inhibitor IκBα and the proto-oncogene product β-catenin by the F-box protein β-TrCP (Pickart, 2001).

Several F-box proteins can recognize short phosphopeptide motifs that correspond to substrate sequences. However, it is unknown whether such interactions are analogous to phosphorylation-dependent interactions of SH2, PTB, 14-3-3, WW and FHA domains, each of which has been crystallized with its cognate phosphopeptide (Yaffe and Elia, 2001). For many SCF substrates, including Sic1, Cdc6 and Cln2, phosphorylation on multiple dispersed sites is required for recognition and degradation (Patton et al., 1998). We recently defined a high affinity consensus phosphopeptide binding motif for Cdc4, termed the Cdc4 phospho-degron (CPD), which bears the consensus I/L-I/L/P-pT-P-<KR>$_4$ [SEQ ID NO:1], where < > indicates a disallowed residue (Nash et al., 2001). The P0 phospho-threonine residue, or less favorably a phospho-serine residue, and the P+1 proline are essential for interaction with Cdc4. Unexpectedly, the CPD consensus is at odds with the CDK phosphorylation site consensus, S/T-P-X-K/R [SEQ ID NO:2](Endicott et al., 1999). Thus, substrate recognition by the targeting kinase is counter-balanced against the targeting component of the degradation machinery. All nine CPD sites in Sic1 have one or more sub-optimal features: all lack consensus hydrophobic residues in the P-1 or P-2 positions, four have serine in place of threonine in the P0 position, and seven contain a disfavored basic residue in one of the +2 to +5 positions. Unexpectedly, Sic1 must be phosphorylated on at least six of its nine sites in order to allow recognition by Cdc4 (Nash et al., 2001). This requirement for multi-site phosphorylation in principle renders the rate of Sic1 degradation proportional to the sixth power of G1 CDK concentration (Ferrell, 1996). The inherently ultrasensitive nature of the Sic1 degradation reaction appears critical for the coordinated initiation of DNA replication by S phase CDK activity (Nash et al., 2001; Lengronne and Schwob, 2002).

The mechanism of the ubiquitin conjugation reaction is not well understood. The ability of E2-E3 enzyme complexes to form polymers of ubiquitin, itself an 8 kDa protein, on a protein substrate presumably demands a large catalytic cradle simply to accommodate the initial reactants (Pickart, 2001). The sequential addition of ubiquitin moieties onto the substrate must also entail considerable flexibility of the substrate and/or the enzyme complex in order to extend the ubiquitin chain. Recent structure determination and modeling of three E2-E3 complexes has provided insight into these issues. A complex of the E2 enzyme UbcH7 and the HECT domain enzyme E6AP reveals a distance of ~ 50Å between the E2 and E3 active sites, suggesting that catalytic transfer of ubiquitin requires large scale movements in an as yet undefined process (Huang et al., 1999). Similarly, a complex between UbcH7 and the RING domain E3 c-Cbl contains a substantial gap between the E2 active site and the substrate binding site on c-Cbl (Zheng et al., 2000). Structures of the SOCS-box adapter protein VHL in complex with a hydroxylated substrate peptide have recently been solved (Kaelin, 2002), but the orientation of the substrate binding site with respect to the E2 enzyme is unknown. Finally, structure determination and molecular modeling of the holo-SCF^{Skp2} complex again suggests a distance of ~ 50Å between the substrate binding LRR domain in Skp2 and the E2 active site (Zheng et al., 2002). Notably, the extensive interdigitation of the Skp1-Skp2 interface and the Skp2 inter-domain interface rigidly fixes the orientation of the LRRs of Skp2, suggesting that the F-box protein might hold the substrate in a very precise orientation with respect to the E2 enzyme (Schulman et al., 2000). However, because the substrate binding site on

Skp2 has not been determined, either by mutation or by co-crystallization with substrate peptide, it is not possible to deduce how SCF substrates might be positioned with respect to the E2 catalytic site.

SUMMARY OF THE INVENTION

Applicants have determined the structures of binding pockets of SCF E3 ubiquitin ligases involved in substrate recognition and/or orientation. More particularly, Applicants have solved the x-ray crystal structure of binding pockets of F-box proteins/ F-box protein-Skp1 complexes of SCF E3 ubiquitin ligases that interact with Cdc4 phospho-degron (CPD) motifs.

Solving the crystal structure has enabled the determination of key structural features of substrate binding pockets of a SCF E3 ubiquitin ligase, particularly the shape of binding pockets, or parts thereof, that permit association of a substrate with a SCF E3 ubiquitin ligase or part thereof. The crystal structure also enables the determination of key structural features in substrates or ligands that interact or associate with the binding pockets.

Knowledge of the structural features of substrate binding pockets of a SCF E3 ubiquitin ligase is of significant utility in drug discovery. The SCF E3 ubiquitin ligase substrate interaction is the basis of many biological mechanisms. In particular it is the basis for regulated ubiquitin proteolysis resulting in degradation of regulatory proteins involved in signaling, development, and cell cycle progression. In addition, drugs may exert their effects through association with the binding pockets of SCF E3 ubiquitin ligases. The associations may occur with all or any parts of a binding pocket. An understanding of the association of a drug with binding pockets of SCF E3 ubiquitin ligases will lead to the design and optimization of drugs having more favorable associations with their targets and thus provide improved biological effects. Therefore, information about the shape and structure of substrate binding pockets of SCF E3 ubiquitin ligases is invaluable in designing potential modulators of the SCF E3 ubiquitin ligases for use in treating diseases and conditions associated with or modulated by the SCF ubiquitin ligases, including cancer and Alzheimer's Disease.

The present invention relates to an isolated binding pocket of an SCF E3 ubiquitin ligase involved in substrate recognition and/or orientation. In an embodiment, the invention relates to a binding pocket of an F-box protein/F-box protein-Skp1 complex of a SCF E3 ubiquitin ligase that interacts with a Cdc4 phospho-degron (CPD) motif. In an aspect of the invention, the binding pocket regulates the binding of a CPD motif to a SCF E3 ubiquitin ligase.

In an embodiment, the invention comprises the structure of a WD repeat domain of an F-box protein. The structure may also comprise a helical linker of an F-box protein and optionally an F-box domain of an F-box protein. Still further the structure may comprise a Skp1 protein.

The invention also relates to a crystal comprising a binding pocket of a SCF E3 ubiquitin ligase involved in substrate recognition and/or orientation.

In an embodiment, the invention provides a crystal comprising a WD repeat domain of an F-box protein. The crystal may also comprise a helical linker of an F-box protein and optionally an F-box domain of an F-box protein. Still further the crystal may comprise a Skp1 protein.

The present invention also contemplates molecules or molecular complexes that comprise all or parts of either one or more binding pockets of the invention, or homologs of these binding pockets that have similar structure and shape.

The invention also contemplates a crystal comprising a binding pocket of a SCF E3 ubiquitin ligase involved with substrate recognition and/or orientation in association with a substrate (e.g. CPD motif). A substrate may be complexed or associated with a binding pocket. The invention further contemplates a crystal comprising a binding pocket of a SCF E3 ubiquitin ligase involved with substrate recognition and/or orientation in association with a ligand. A ligand may be a modulator of the activity of a SCF E3 ubiquitin ligase. A ligand may be complexed or associated with a binding pocket

In an aspect the invention contemplates a crystal comprising a binding pocket of an SCF E3 ubiquitin ligase involved in substrate recognition and/or orientation complexed with a substrate from which it is possible to derive structural data for the substrate.

The shape and structure of a binding pocket may be defined by selected atomic contacts in the pocket. In an embodiment, the binding pocket is defined by one or more atomic interactions or enzyme atomic contacts as set forth in Table 3 or Table 4. Each of the atomic interactions is defined in Table 3 or Table 4 by an atomic contact (more preferably, a specific atom where indicated) on the F-box protein and by an atomic contact (more preferably a specific atom where indicated) on the substrate. The atomic interactions are also defined by an atomic contact on one portion of the F-box protein and an atomic contact on another portion of the F-box protein.

An isolated polypeptide comprising a binding pocket with the shape and structure of a binding pocket described herein is also within the scope of the invention.

The invention also provides a method for preparing a crystal of the invention, preferably a crystal of a binding pocket of an SCF E3 ubiquitin ligase involved in substrate recognition and/or orientation, or a complex of such a binding pocket and a substrate.

Crystal structures of the invention enable a model to be produced for a binding pocket of the invention, or complexes or parts thereof. The models will provide structural information about the interactions of a substrate or ligand with a binding pocket. Models may also be produced for substrates and ligands. A model and/or the crystal structure of the present invention may be stored on a computer-readable medium.

The present invention includes a model of a binding pocket of the present invention that substantially represents the structural coordinates specified in Table 6 or portions thereof. The invention also includes a model that comprises modifications of the structure substantially represented by the structural coordinates specified in Table 6. A model is a representation or image that predicts the actual structure of the binding pocket. As such, a model is a tool that can be used to probe the relationship between a binding pocket's structure and function at the atomic level, and to design molecules that can modulate the binding site and accordingly activity of an F-box protein or SCF complex.

Thus, the invention provides a model of: (a) a binding pocket of an SCF E3 ubiquitin ligase involved in substrate recognition and/or orientation; and (b) a modification of the model of (a).

A method is also provided for producing a model of the invention representing a binding pocket of an SCF E3 ubiquitin ligase involved in substrate recognition and/or orientation, comprising representing amino acids of the binding pocket at substantially the structural coordinates specified in Table 6.

A crystal and/or model of the invention may be used in a method of determining the secondary and/or tertiary structures of a polypeptide or binding pocket with incompletely characterised structure. Thus, a method is provided for determining at least a portion of the secondary and/or tertiary structure of molecules or molecular complexes which contain at least some structurally similar features to a binding pocket of the invention. This is achieved by using at least some of the structural coordinates set out in Table 6.

A crystal of the invention may be useful for designing, modeling, identifying, evaluating, and/or synthesizing mimetics of a binding pocket or ligands or substrates that associate with a binding pocket. Such mimetics or ligands may be capable of acting as modulators of an F-box protein or SCF E3 ubiquitin ligase activity, and they may be useful for treating, inhibiting, or preventing diseases modulated by such a protein or ligase.

Thus, the present invention contemplates a method of identifying a modulator of a F-box protein or an SCF E3 ubiquitin ligase comprising the step of applying the structural coordinates of a binding pocket, or atomic interactions, or atomic contacts of a binding pocket, to computationally evaluate a test ligand or substrate for its ability to associate with the binding pocket, or part thereof. Use of the structural coordinates of a binding pocket, or atomic interactions, or atomic contacts of a binding pocket to design or identify a modulator is also provided.

In an embodiment, the invention contemplates a method of identifying a modulator of an F-box protein or an SCF E3 ubiquitin ligase comprising determining if a test agent inhibits or potentiates the interaction of an F-box protein or SCF E3 ubiquitin ligase with its substrate.

The invention further contemplates classes of modulators of F-box proteins or SCF E3 ubiquitin ligases based on the shape and structure of a ligand or substrate defined in relation to the molecule's spatial association with a binding pocket of the invention. Generally, a method is provided for designing potential inhibitors of an F-box protein-substrate interaction or SCF E3 ubiquitin ligase–substrate interaction comprising the step of applying the structural coordinates of a substrate or ligand defined in relation to its spatial association with a binding pocket, or a part thereof, to generate a compound that is capable of associating with the binding pocket.

It will be appreciated that a modulator of an F-box protein or SCF E3 ubiquitin ligase may be identified by generating an actual secondary or three-dimensional model of a binding pocket, synthesizing a compound, and examining the components to find whether the required interaction occurs.

A potential modulator of an F-box protein or SCF E3 ubiquitin ligase identified by a method of the present invention may be confirmed as a modulator by synthesizing the compound, and testing its effect on the F-box protein or SCF E3 ubiquitin ligase in an assay.

A modulator of the invention may be converted using customary methods into pharmaceutical compositions. A modulator may be formulated into a pharmaceutical composition containing a modulator either alone or together with other active substances.

Therefore, the methods of the invention for identifying modulators may comprise one or more of the following additional steps:

(a) testing whether the modulator is a modulator of the activity of an F-box protein or an SCF E3 ubiquitin ligase, preferably testing the activity of the modulator in cellular assays and animal model assays;

(b) modifying the modulator;

(c) optionally rerunning steps (a) or (b); and

(d) preparing a pharmaceutical composition comprising the modulator.

Steps (a), (b) (c) and (d) may be carried out in any order, at different points in time, and they need not be sequential.

Still another aspect of the present invention provides a method of conducting a drug discovery business comprising:

(a) providing one or more systems employing the atomic interactions, atomic contacts, or structural coordinates of a binding pocket of an F-box protein or SCF E3 ubiquitin ligase involved in substrate recognition and/or orientation, for identifying agents by their ability to inhibit or potentiate the atomic interactions or atomic contacts of a binding pocket;

(b) conducting therapeutic profiling of agents identified in step (a), or further analogs thereof, for efficacy and toxicity in animals; and

(c) formulating a pharmaceutical preparation including one or more agents identified in step (b) as having an acceptable therapeutic profile.

A further aspect of the present invention provides a method of conducting a drug discovery business comprising:

(a) providing one or more systems for identifying agents by their ability to inhibit or potentiate the interaction between an F-box protein or SCF complex and its substrate; and

(b) conducting therapeutic profiling of agents identified in step (a), or further analogs thereof, for efficacy and toxicity in animals; and

(c) formulating a pharmaceutical preparation including one or more agents identified in step (b) as having an acceptable therapeutic profile.

In certain embodiments, the subject methods can also include a step of establishing a distribution system for distributing the pharmaceutical preparation for sale, and may optionally include establishing a sales group for marketing the pharmaceutical preparation.

Yet another aspect of the invention provides a method of conducting a target discovery business comprising:

(a) providing one or more systems employing the atomic interactions, atomic contacts, or structural coordinates of a binding pocket of an F-box protein or SCF complex involved in substrate

recognition and/or orientation, for identifying agents by their ability to inhibit or potentiate the atomic interactions or atomic contacts;

(b) (optionally) conducting therapeutic profiling of agents identified in step (a) for efficacy and toxicity in animals; and

(c) licensing, to a third party, the rights for further drug development and/or sales for agents identified in step (a), or analogs thereof.

Methods are also provided for regulating an F-box protein – substrate interaction or an SCF E3 ubiquitin ligase–substrate interaction by changing a binding pocket involved in substrate recognition and/or orientation. A binding pocket may be changed by altering amino acid residues forming the binding pocket (e.g. introducing mutations) or using a modulator.

The invention also contemplates a method of treating or preventing a condition or disease associated with an F-box protein or an SCF E3 ubiquitin ligase in a cellular organism, comprising:

(a) administering a modulator of the invention in an acceptable pharmaceutical preparation; and

(b) potentiating or inhibiting the F-box protein or SCF E3 ubiquitin ligase to treat or prevent the disease.

In an embodiment the condition or disease is cancer or Alzheimer's disease.

The invention provides for the use of a modulator identified by the methods of the invention in the preparation of a medicament to treat or prevent a disease in a cellular organism. Use of modulators of the invention to manufacture a medicament is also provided.

These and other aspects of the present invention will become evident upon reference to the following detailed description and Tables, and attached drawings.

DESCRIPTION OF THE DRAWINGS AND TABLES

The present invention will now be described only by way of example, in which reference will be made to the following Figures:

Figure 1 shows structure based sequence alignments of (A) Skp1 orthologs and (B) Cdc4 orthologs (red) and paralogs (black). Human Fbw7 and β-TrCP1 are isoforms 1 and 2, respectively. Secondary structure elements are colored as in Figure 2A. Disordered regions in the crystal structure are shown as dashed lines. Red residues are essential for the Cdc4 function, blue residues strongly influence but do not abrogate function, green residues are non-essential but conserved around the binding pocket, and yellow residues are conserved elsewhere. Circles indicate mutations associated with excessive cell proliferation in flies and/or cancer in humans. Deletion of residues 37-64 in Skp1 is denoted by a triangle and a replacement of two closely placed loops from residues 602-605 and 609-624 is denoted by the underline of the short interloop sequence Gly-Glu-Leu. Insertions to optimize sequence alignments are indicated by number of residues inserted in gray. The non-standard β-strand element 9^1 in ScCdc4 is marked by the red asterisk and is shown in full at the bottom of the alignment. Residues that anchor helix α6 to the F-box domain are

marked by green hearts, those that anchor helix α6 to the WD40 domain by red hearts and those that make direct contact between the WD40 domain and F-box domain by blue asterisks. [SEQ ID NOs 3-16.]

Figure 2 shows an overview of the Skp1-Cdc4-CPD complex. (A) Ribbon representation of Skp1 and the F-box domain (274-319), the helical linker region (331-366), and the WD40 domain of Cdc4 (367-744) coloured green, red, pink, and blue, respectively. The bound cyclin E derived CPD peptide is shown in purple with the phospho-threonine moiety shown in ball and stick representation. Secondary structure elements are indicated. Positions of disordered loop regions are shown as ribbon breaks. All ribbons representations were generated using Ribbons. (B) Ribbons representation highlighting the WD 40 domain of Cdc4. β propeller blades are denoted PB1 to PB8, and the component secondary structure elements are indicated. Ribbons and CPD peptide are coloured as in (A). Position of the WD40 domain is identical to that in Figures 4A to 4C. (C) The structured linkage between the WD40 domain and the F box domain of Cdc4.

Figure 3 shows an overview of the CPD binding region of the Ccdc4 WD40 repeat domain. (A) Molecular surface representation of the CPD binding pocket indicating invariant and highly conserved residues. Basic, hydrophobic and small residues are coloured blue, green and orange respectively. The bound CPD is shown in ball and stick representation with carbon, nitrogen, oxygen and phosphorous atoms coloured white, blue, red and yellow respectively. All surface representation were generated using Grasp. (B) Surface representation of CPD binding region as oriented in (A) coloured according to electrostatic potential. Blue and red indicate regions of positive and negative potential respectively (10 to -10 k_BT). Residues of the bound CPD are labeled. (C) Stereo ribbons representation highlighting side chains and molecular interactions in the CPD binding pocket. CPD residues and highly conserved and invariant Cdc4 residues are displayed in ball and stick representation. Sites of mutation that give rise to severe loss of function are coloured red, and intermediate loss of function are coloured yellow (see Table 5). All other highly conserved and invariant residues are coloured green. Reference propeller blades of the WD40 repeat domain are indicated. (D) Stereo ribbons representation of the CPD binding pocket highlighting cancer causing mutations in drosophila and human Cdc4 orthologues. Arginine mutations in H-cell lines or entrometrial cells are coloured red. Drosophila mutations are coloured blue and Cdc4 temperature sensitive mutations (Rosamond personal communication) are coloured yellow. (E) Multiple Anomalous Dispersion phased electron density map corresponding to the CPD bound to the WD40 repeat domain of Cdc4. Refined CPD model is shown in ball and stick representation. Figure generate using O. (F) Schematic of CPD binding pocket interactions with the CPD peptide.

Figure 4 shows (A) Stereo ribbons representation of the human Skp1-Skp2 complex superimposed on the yeast Skp1-Cdc4-CPD complex. Human Skp1-Skp2 and yeast Skp1-Cdc4 were superimposed through a least squares optimization of Skp1β strands 1 to 3 and α-helices 1 to 6 (RMSD = 0.74Å). The yeast Skp1-Cdc4 complex is coloured as in Figure 2. Human Skp1, the Skp2 F-box, and the Skp2 Leucine-rich repeat domain are coloured orange, green, and light blue, respectively. Skp1 and F box secondary structure elements that deviate significantly in size and position between the two structures are labeled. (B) Model of the $SCF^{Cdc4\text{-}CPD}$ E2 complex. The yeast Skp1-Cdc4-CPD complex is coloured as in Figure 2. Cul1, Rbx1, and E2 proteins are coloured pink, red, and light blue, respectively.

The arrow indicates the distance between the peptide binding site and the active site cysteine of the E2. The structure was generated using the ternary complex of the cullin cdc53, rbx1, Skp1, previously reported, and superimposing the E2 structure from the E2/Cbl ring finger structure and the structure of Skp1, Cdc4 and a phosphorylated CPD peptide

Figure 5 shows (A) Selection of Sic1 phosphoisoforms by wild type and mutant forms of Cdc4. (B) In vitro ubiquitination of Sic1 isoforms by wild type and mutant SCFCdc4 complexes. (C) Natural CPD sites deviate from the optimal CPD by one or more or more residues.

Figure 6 shows substrate orientation within the Skp1-Cdc4-CPD complex.(A) Comparison of the ScSkp1–ScCdc4–CPD complex and the hSkp1–hSkp2 complex. Complexes were superimposed through a least squares optimization of Skp1 β-strands 1 to 3 and α-helices 1 to 6 (RMSD Cα= 0.74Å). Skp1 and F-box secondary structure elements that deviate significantly in size and position between the two structures are labeled. (B) Model of the ubiquitin–E2–SCF^{Cdc4}–CPD complex. The arrow indicates the 59Å distance separating the phosphate group of the CPD and the active site cysteine of the E2.

Figure 7 shows the CPD binding pocket of the WD40 domain. (A) Surface representation of the CPD binding pocket indicating invariant and highly conserved residues. Basic (blue), hydrophobic (green) and small polar residues (orange) are shown. The bound CPD is in ball and stick representation with carbon (white), nitrogen (blue), oxygen (red) and phosphorous (yellow) atoms shown. (B) Surface representation of CPD binding region indicating electrostatic potential. Blue and red indicate regions of positive and negative potential, respectively, over the range 10 to −10 k_BT. (C) Stereo ribbons representation of side chains and molecular interactions in the CPD binding pocket. Highly conserved and invariant side chains of Cdc4 and the CPD are displayed in ball and stick representation. Sites of mutation that give rise to severe and intermediate loss of function (see Figure 8) are colored red and blue, respectively; non-essential residues are colored green.

(D) Schematic of CPD binding pocket interactions with the CPD peptide.

Figure 8 shows structure-guided mutational analysis of Cdc4. (A) Residues required for interaction of phospho-Sic1 and Cdc4 in vitro. Sic1 was phosphorylated with Cln2-Cdc28 kinase and captured onto resin loaded with either wild type or the indicated mutant forms of Skp1–Cdc4 complex. (B) Residues essential for Cdc4 function in vivo. Complementation of a *cdc4Δ* strain by the indicated alleles was assessed in a plasmid shuffle assay. The R485A, R467A and R534A mutations in Cdc4 have been previously shown to disrupt function in vivo (Nash et al., 2001) and so are not shown. (C) Effect of Cdc4 mutations on sensitivity to increased *SIC1* dosage. Strains bearing indicated *CDC4* alleles were tested for sensitivity to overexpression of wild type *SIC1* and a partially stabilized version, $SIC1^{Thr33Val}$ from the *GAL1* promoter. Strains were incubated on galactose or glucose medium for 2 days at 30°C.

Figure 9 shows the modulation of the multisite requirement for phospho-Sic1-Cdc4 interaction. (A) All natural CPD sites in Sic1 deviate from the CPD consensus. Underlined residues indicate sub-optimal residues at the P-1 and P-2 positions, boxed residues indicate sub-optimal basic residues at the P+2 to P+5 positions and asterisks indicate a sub-optimal pSer at the P0 position. (B) Capture of Sic1 phospho-isoforms by wild type and mutant Cdc4.

Pools of differentially phosphorylated Sic1 were captured on Skp1–Cdc4 resin, using either wild type or the indicated mutant forms of Cdc4 compromised for selection at the P-1 position (V384N W717N) or the P+2 to P+5 positions (K402A R443D). The input and bound phospho-Sic1 isoform pools were resolved by denaturing IEF-2D gel electrophoresis and visualized by anti-Sic1 immunoblot. (C) Ubiquitination of phospho-Sic1 isoforms by wild type and mutant SCF^{Cdc4} complexes. Pools of differently phosphorylated Sic1 were incubated in solution with an equimolar amount of the indicated SCF^{Cdc4} complexes, Cdc34, ubiquitin and ATP for 1 h at 30°C. Input and reaction products were separated and visualized as in (B). Arrows indicate the less phosphorylated forms of Sic1 captured by Cdc4 selection mutants. Asterisk indicates more extensively ubiquitinated species (D) Possible interaction mechanisms for single site and multi-site dependent substrate binding to Cdc4. In a two-site cooperative interaction model (left), a primary high affinity CPD binding site acts in conjunction with a secondary weak CPD binding site. The free energy for the two interactions is additive and so the overall K_d increases multiplicatively. In a single-site allovalent interaction (right), multiple low affinity CPD sites engage a single CPD binding site on Cdc4 in equilibrium. The high local concentration of CPD sites increases the probability of binding such that Sic1 is unable to diffuse away from Cdc4 before re-binding occurs. The probability of re-binding increases as an exponential function of the number of CPD sites, thus accounting for the apparent cooperativity of the interaction.

The present invention will now be described only by way of example, in which reference will be made to the following Tables:

Table 1 shows data collection, structure determination and refinement statistics of a crystal of the invention.

Table 2 shows data collection, structure determination and refinement statistics of a crystal of the invention.

Table 3 shows intermolecular contacts in a binding pocket of the invention.

Table 4 shows intermolecular contacts in a binding pocket of the invention.

Table 5 shows mutant cdc4 polyppeptides of the invention. Mutational analysis of the CPD binding surface. Mutants were tested *in vitro* by ability to bind phosphorylated Sic1 and then captured onto GST-Skp1/Cdc4 resin and detected with anti-sic1 antibody. Mutants were tested *in vivo* by ability to degrade GAL1-SIC1 or various phosphorylation mutants. Sites are as follows: 3 = Thr 33, Thr 45, Ser 76; 4 = Thr 5, Thr 33, Thr 45, Ser 76; 5 = Thr 2, Thr 5, Thr 33, Thr 45, Ser 76; 6 = Thr 2, Thr 5, Thr 33, Thr 45, Ser 69, Ser 76; 7 = Thr 2, Thr 5, Thr 33, Thr 45, Ser 69, Ser 76, Ser 80. GAL1-SIC1 plasmids were transformed into a cdc4Δ strain containing a copy of CDC4 on a TRP1 ARS CEN plasmid. Strains were incubated for 2 days at 30°C.

Table 6 shows the structural coordinates of a binding pocket of the invention.

In Table 6, from the left, the second column identifies the atom number; the third identifies the atom type; the fourth identifies the amino acid type; the sixth identifies the residue number; the seventh identifies the x coordinates; the eighth identifies the y coordinates; the ninth identifies the z coordinates; the tenth identifies the occupancy; and the eleventh identifies the temperature factor.

Table 7 lists the oligonucleotides used in the studies described in the examples.

Table 8 lists the plasmids used in the studies described in the examples.

DETAILED DESCRIPTION OF THE INVENTION

In accordance with the present invention there may be employed conventional molecular biology, microbiology, and recombinant DNA techniques within the skill of the art. Such techniques are explained fully in the literature. See for example, Sambrook, Fritsch, & Maniatis, Molecular Cloning: A Laboratory Manual, Second Edition (1989) Cold Spring Harbor Laboratory Press, Cold Spring Harbor, N.Y); DNA Cloning: A Practical Approach, Volumes I and II (D.N. Glover ed. 1985); Oligonucleotide Synthesis (M..J. Gait ed. 1984); Nucleic Acid Hybridization B.D. Hames & S.J. Higgins eds. (1985); Transcription and Translation B.D. Hames & S.J. Higgins eds (1984); Animal Cell Culture R.I. Freshney, ed. (1986); Immobilized Cells and enzymes IRL Press, (1986); and B. Perbal, A Practical Guide to Molecular Cloning (1984).

GLOSSARY

Abbreviations for amino acid residues are the standard 3-letter and/or 1-letter codes used in the art to refer to one of the 20 common L-amino acids. Likewise abbreviations for nucleic acids are the standard codes used in the art.

" Skp1-Cdc53/Cullin-F-box protein (SCF) E3 ubiquitin ligases" or "SCF complex" refers to a protein complex comprising the adaptor protein Skp1, the scaffold protein cdc53/cullin, a RING-H2 domain protein Rbx1 (also called Roc1 or Hrt1), and an F-box protein, which protein complex augments or otherwise facilitates the ubiquitination of a protein. In certain aspects of the present invention an SCF complex refers to a complex comprising Skp1 and an F box protein or parts thereof.

In the context of the present invention the term "F-box protein" refers to a protein comprising a characteristic structural motif called the F-box as described in Bai et al, (1996 *Cell* 86: 263-274) and a protein-protein interaction domain, in particular a WD40 repeat motif or domain. Examples of F-box Proteins include Cdc4 polypeptides, and homologs or portions thereof, preferably portions that interact with a CPD motif (e.g. WD repeat).

A "WD40 repeat", "WD40 motif", or "WD repeat domain" is generally defined as a contiguous sequence of about 25 to 50 amino acids with relatively-well conserved sets of amino acids [i.e. Trp-Asp (WD)] at the ends (amino- and carboxyl- terminal) of the sequence. (For reviews see Neer EJ, Schmidt CJ, Nambudripad R & Smith TF: "The ancient regulatory-protein family of WD-repeat proteins," Nature 371, 297-300 (1994) PMID: 8090199; and Smith TF, Gaitatzes CG, Saxena K & Neer EJ: "The WD-repeat: a common architecture for diverse functions," TIBS 24, 181-185 (1999) PMID: 10322433.) A WD repeat motif or domain can also be defined as a domain of an F-box protein that interacts with a CPD motif or like motif.

Examples of WD-repeat-containing proteins are cdc4 polypeptides, Met30 homologues and orthologues (see for example, GenBank Accession No. P39014 or MT30_YEAST - SEQ ID NO.17) and β-TRCP homologues and orthologues (see for example, GenBank Accession No. NP_033901 - SEQ ID NO.18). Other WD40 repeat-containing proteins will, however, be appreciated by those skilled in the art. A WD40-repeat protein also includes a part of the protein. A person skilled in the art may conduct searches to identify proteins that contain WD-40 repeats, in particular F-box proteins. For example, on-line databases such as GenBank or SwissProt can be searched, either with an entire sequence of a WD-40-containing protein, or with a consensus WD-40 repeat sequence. Various search algorithms

and/or programs may be used, including FASTA, BLAST or ENTREZ. FASTA and BLAST are available as a part of the GCG sequence analysis package (University of Wisconsin, Madison, Wis.). ENTREZ is available through the National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health, Bethesda, Md. The number of WD-40 repeats in a particular protein can range from two to more than eight.

A "Cdc4 Phospho-Degron motif" or "CPD motif" is a motif that targets substrates for ubiquitination by SCF complexes. The motif can be defined by the consensus sequence X^2-X^3-pThr-Pro-X^4 (SEQ ID NO.19), more particularly X^2-X^3-pThr-Pro-X^4-X^5-X^6-X^7 (SEQ ID NO.20), wherein X^2 represents Leu, Pro, or Ile, preferably Leu or Ile; X^3 represents Leu, Ile, Val, or Pro, preferably Ile, Leu, or Pro; X^4 represents any amino acid except basic and bulky hydrophobic amino acids, preferably X^4, X^5 and X^6 represent any amino acid except basic and bulky hydrophobic amino acids, preferably X^4 is any amino acid except Arg, Lys, Tyr, or Trp, more preferably X^4 is Ile, Val, Pro, or Gln, preferably X^5 and X^6 are any amino acid except Arg, Lys, or Tyr and more preferably X^5 is Gln, Leu, Met, Thr, or Glu, and X^6 is Gln, Ala, Thr, Glu, or Ser; and X^7 is any amino acid, preferably not a basic or bulky hydrophobic amino acid, more preferably X^7 is any amino acid except Arg, Lys, or Tyr, most preferably X^7 is Leu, Trp, Asp, Pro, or Gly. A CPD motif preferably comprises the consensus sequence -Leu/Gly/Tyr-Pro-pThr-Pro- (SEQ ID NO.21).

A CPD motif containing protein includes proteins comprising the CPD motif including but not limited to Gcn4, Cyclin E, Far1, Ash1, Sic1, Pc17, Cdc16, $p27^{kip1}$, Cln2, and transcription factors such as β catenin or Iκβα, and homologues of these proteins. The term includes but is not limited to all homologs, orthologs, naturally occurring allelic variants, isoforms and precursors of the polypeptides. Other proteins containing CPD motif sequences may be identified with a protein homology search, for example by searching available databases such as GenBank or SwissProt and various search algorithms and/or programs may be used including FASTA, BLAST (available as a part of the GCG sequence analysis package, University of Wisconsin, Madison, Wis.), or ENTREZ (National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health, Bethesda, MD).

The term "substrate" refers to a protein that interacts with an F-box protein targeting it for ubiquitin-dependent proteolysis, or a protein targeted for F-box dependent degradation. Examples of substrates are CPD motif containing proteins including Gcn4, CyclinE, Far1, Ash1, Sic1, Pc17, Cdc16, $p27^{kip1}$; Cln2, and, transcription factors such as β catenin or Iκβα. The term also refers to a part of a protein that interacts with an F-box protein, including a CPD motif, and analogues of substrates or parts thereof

A "ligand" refers to a compound or entity that associates with a binding pocket, or modulators of an F-box protein or SCF E3 ubiquitin ligase, including inhibitors. A ligand may be designed rationally by using a model according to the present invention.

The terms "cdc4 polypeptide" is used to refer to polypeptides of the cdc4 family of proteins characterized by an F-box motif and WD repeats. The term includes but is not limited to all homologs, orthologs, naturally occurring allelic variants, isoforms and precursors of the polypeptides of GenBank Accession Nos. S56245 or SEQ ID NO. 22 (*Saccharomyces cerevisiae* cdc4), CAA65538 or SEQ ID NO. 23 (*Candida albicans* cdc4), AAL07271 or SEQ ID

NO. 24 (human cdc4), AAC47809 or SEQ ID NO. 25 (sel-10), AAK57547 or SEQ ID NO. 26 (*Homo sapiens* F-box protein FBW7), and AAG09623F or SEQ ID NO. 27 (*Homo sapiens* F box protein FBX30). In general, for example, naturally occurring allelic variants will share significant homology (70-90%) to these sequences. Allelic variants may contain conservative amino acid substitutions from cdc4 sequences or will contain a substitution of an amino acid from a corresponding position in a cdc4 homologue such as, for example, the human homologue. [See Strohmaier,H., Nature 413 (6853), 316-322 (2001) for a description and sequence of human cdc4]. The term also includes the mutant cdc4 polypeptides described herein. Figure 1 shows a structure based sequence alignment of cdc4 orthologs and paralogs.

The term "cdc53" or "cdc53 polypeptide" is used interchangeably herein with the term "cullins" when referring to a vertebrate homolog of the yeast cdc53 protein. The term "cullin polypeptide" or "cullin protein", refers to a member of the cullins family, e.g., any one of cul-1, -2, -3, -4, -5, or -6. The term includes but is not limited to all homologs, naturally occurring allelic variants, isoforms and precursors of a cdc53 polypeptide or cullin of GenBank Accession Nos. AAB38821 or SEQ ID NO. 28 (*Saccharomyces cerevisiae* cdc53), AAC36304 or SEQ ID NO. 29 (*Homo sapiens* cullin 3), AAC51190 or SEQ ID NO. 30 (*Homo sapiens* cullin 2), NP_ 003581 or SEQ ID NO. 31 (Homo sapiens cullin 3), AF126404_1 or SEQ ID NO. 32 (Homo sapiens cullin 2), CUL1_CAEEL or SEQ ID NO. 33 (*Caenorhabditis elegans* cullin 1), AAA85085 or SEQ ID NO. 34 (*Drosophila melanogaster* cullin 1) and the cullins described in Kipreos ET (Cell 1996 Jun 14;85(6):829-39). In general for example, naturally occurring allelic variants of cdc53 will share significant homology (70-90%) to the cdc53 or cullin sequences. Allelic variants may contain conservative amino acid substitutions from the cdc4 sequence or will contain a substitution of an amino acid from a corresponding position in a cdc4 homolog such as, for example, the human homolog.

The term "Skp1" or "Skp1 polypeptide" is used to refer to polypeptides that connect cell cycle regulators to the ubiquitin proteolysis machinery by associating with F-box proteins through the F-box motif. The term includes but is not limited to all homologs, naturally occurring allelic variants, isoforms and precursors of Skp1 of GenBank Accession Nos. SKP1_SCHPO or SEQ ID NO. 35 (*Schizosaccharomyces pombe*), BAB62325 or SEQ ID NO. 36 (*Schizosaccharomyces pombe*), AAC49492 or SEQ ID NO. 37 (*Saccharomyces cerevisiae*), and AAB17500 or SEQ ID NO. 38 (*Saccharomyces cerevisiae*). In general, for example, naturally occurring allelic variants of Skp1 will share significant homology (70-90%) to the Skp1 sequences. Allelic variants may contain conservative amino acid substitutions from the Skp1 sequence or will contain a substitution of an amino acid from a corresponding position in a Skp1 homolog such as, for example, the human homolog. Figure 1 shows a structure based sequence alignment of Skp1 homologues.

A CPD motif and WD repeat or proteins containing same, cdc4 polypeptides, cdc53, Skp1, substrates, and SCF complexes, may be from any species, particularly a mammalian species, including bovine, ovine, porcine, murine, equine, preferably the human species, and from any source, whether natural, synthetic, semi-synthetic, or recombinant.

The term "agonist" of a binding pocket refers to a compound or ligand that interacts with the binding pocket and maintains or increases the activity of the binding pocket to which it binds. The term includes partial agonists and inverse agonists. Agonists may include proteins, peptides, nucleic acids, carbohydrates, or any other molecules that bind to a binding pocket. Agonists also include a molecule derived from a binding pocket. Peptide mimetics, synthetic molecules with physical structures designed to mimic structural features of particular peptides, may serve as agonists. The stimulation may be direct, or indirect, or by a competitive or non-competitive mechanism. The term includes partial agonists and inverse agonists.

As used herein, the term "partial agonist" means an agonist that is unable to evoke the maximal response of a biological system, even at a concentration sufficient to saturate the specific receptors.

As used herein, the term "partial inverse agonist" is an inverse agonist that evokes a submaximal response to a biological system, even at a concentration sufficient to saturate the specific receptors. At high concentrations, it will diminish the actions of a full inverse agonist.

The term "antagonist", as used herein, refers to a ligand or compound that binds a binding pocket but does not maintain the activity of the binding pocket to which it binds. The term can also includes a ligand that reduces the action of another agent, such as an agonist. An antagonistic action may result from a combination of the substance being antagonised (chemical antagonism) or the production of an opposite effect through a different protein (functional antagonism or physiological antagonism) or as a consequence of competition for the binding site of an intermediate that links a protein to the effect observed (indirect antagonism). The antagonist may act at the same site as the agonist (competitive antagonism). Antagonists may include proteins, peptides, nucleic acids, carbohydrates, or any other molecules that bind to a binding pocket. Antagonists also include a molecule derived from a binding pocket. Peptide mimetics, synthetic molecules with physical structures designed to mimic structural features of particular peptides, may serve

As used herein, the term "competitive antagonism" refers to the competition between an agonist and an antagonist for a binding pocket of a protein that occurs when the binding of agonist and antagonist becomes mutually exclusive. This may be because the agonist and antagonist compete for the same binding sites or pockets, or combine with adjacent but overlapping sites. A third possibility is that different sites are involved but that they influence the receptor macromolecules in such a way that agonist and antagonist molecules cannot be bound at the same time. If the agonist and antagonist form only short lived combinations with a binding pocket so that equilibrium between agonist, antagonist and binding pocket is reached during the presence of the agonist, the antagonism will be surmountable over a wide range of concentrations. In contrast, some antagonists, when in close enough proximity to their binding site, may form a stable covalent bond with it and the antagonism becomes insurmountable when no spare receptors remain.

By being "derived from" a binding pocket is meant any molecular entity which is identical or substantially equivalent to the binding pocket. A peptide derived from a binding pocket may encompass the amino acid sequence of a naturally occurring binding pocket, any portion of that binding pocket or other molecular entity that functions to

bind to an associated or interacting binding pocket. A peptide derived from such a binding pocket will interact directly or indirectly with an associated molecule in such a way as to mimic the native binding pocket. Such peptides may include competitive inhibitors, peptide mimetics, and the like. The entity will not include a full length sequence of a wild-type molecule. Peptide mimetics, synthetic molecules with physical structures designed to mimic structural features of particular peptides, may serve as inhibitors or enhancers.

"Peptide mimetics" are structures which serve as substitutes for peptides in interactions between molecules (See Morgan et al (1989), Ann. Reports Med. Chem. 24:243-252 for a review). Peptide mimetics include synthetic structures which may or may not contain amino acids and/or peptide bonds but retain the structural and functional features of a peptide, or agonist or antagonist (i.e. enhancer or inhibitor) of a binding pocket. Peptide mimetics also include peptoids, oligopeptoids (Simon et al (1972) Proc. Natl. Acad, Sci USA 89:9367); and peptide libraries containing peptides of a designed length representing all possible sequences of amino acids corresponding to a motif, peptide, or agonist or antagonist (i.e. enhancer or inhibitor) of the invention.

Sequences are "homologous" or considered "homologs" when at least about 70% (preferably at least about 80 to 90%, and most preferably at least 95%) of the nucleotides or amino acids match over a defined length of the molecule. "Substantially homologous" also includes sequences showing identity to the specified sequence. Percent identity can be determined electronically, e.g., by using the MEGALIGN program (DNASTAR, Inc., Madison Wis.) which can create alignments between two or more sequences according to different methods, e.g., the clustal method. (See, e.g., Higgins, D. G. and P. M. Sharp (1988) Gene 73:237-244.) Percent identity can also be determined by other methods known in the art, (e.g., the Jotun Hein method. (See, e.g., Hein, J. (1990) Methods Enzymol. 183:626-645) or by varying hybridization conditions). Preferably, the amino acid or nucleic acid sequences have an alignment score of greater than 5 (in standard deviation units) using the program ALIGN with the mutation gap matrix and a gap penalty of 6 or greater (Dayhoff).

BINDING POCKET

"Binding pocket" refers to a region or site of an F-box protein or molecular complex thereof (e.g. Skp1-F-box complex, SCF E3 ubiquitin ligase) involved in substrate selection and/or orientation. As the result of its shape, a binding pocket associates with another region of an F-box protein or SCF complex or with a substrate or a part thereof.

In an aspect of the invention a binding pocket comprises one or more of the residues involved in selection and/or orientation of a substrate or ligand.

In an aspect of the invention a binding pocket is provided that comprises the WD40 repeat domain of an F-box protein. In another embodiment the binding pocket comprises a WD40 repeat domain and a helical linker of an F-box protein. In a further embodiment, the binding pocket comprises a WD40 repeat domain, a helical linker and an F-box domain of an F-box protein. In an embodiment the F-box protein is a cdc4 polypeptide or portion thereof.

A binding pocket of the invention may comprise a WD40 repeat domain characterized by one or more of the following characteristics:

(a) a 7 or 8 blade β-propeller structure, in particular a 8 blade β-propeller structure;

(b) a disk like structure characterized by a cavity in the middle and two opposing circular surfaces of different size;

(c) a conical frustum of about 40Å top surface and about 50Å bottom surface, an overall thickness of 30Å and a central pore of 6Å diameter; and

(d) a CPD binding site on the top surface of the frustum of (c) and running across the edge of the pore, while the bottom surface of the frustum links to the F-box domain.

A binding pocket of the invention may be characterized by one or more of the following characteristics:

(i) a dedicated pThr-Pro binding pocket;

(ii) a deep hydrophobic pocket that selects hydrophobic residues N-terminal to the phosphorylation site of a CPD, and

(iii) a through space electrostatic selection against basic residues C-terminal to the phosphorylation site of a CPD.

A binding pocket of the invention may comprise a helical linker characterized by α helices that form a stalk and pedestal like structure that connects and orients a WD repeat domain. The helical linker binding pocket can also be characterized by one or more of the following:

(a) a helix (e.g. α6 in Figure 2 or Figure 6) that is 30Å in length and is anchored at its N-terminus to the hydrophobic core of the F-box/helical extension and at its C-terminus to the hydrophobic core of a WD repeat domain,

(b) the helix of (a) (e.g. α6) anchored at its amino terminus to an F-box through hydrophobic interactions (e.g. involving α6 residues Phe 355, Leu356, and F box residues Ile295, Ile296, Leu315, Leu 319 and Trp316 of Cdc4 or the corresponding residues in Cdc4 homologs, variants, precursors etc.);

(c) a second helix (e.g. helix 5) packed along the base of the helix of (a) or (b) opposite to the F-box domain through hydrophobic interactions (e.g. involving Tyr342, Leu338, and Leu 334 of Cdc4 or the corresponding residues in Cdc4 homologs, variants, precursors etc.);

(d) the helix of (a) (e.g. helix α6) anchored at its C-terminus through hydrophobic interactions;

(e) a C-terminal end of helix α6 inserted obliquely between propeller blades β7 and β8 of a WD40 domain through van der Wals and hydrophobic interactions (e.g. involving Trp365 and Ile361 with WD40 domain residues Val687, Ile696, Leu726, and Phe743 in β-propeller blades 7 and 8 of Cdc4 or the corresponding residues in Cdc4 homologs, variants, precursors etc.).

A CPD motif binding pocket of the invention may comprise a hydrophobic pocket that surrounds the open central channel of a 7 or 8 blade WD repeat propeller. A binding pocket of Cdc4 is more particularly characterized by one or more of the following:

(a) a WD repeat domain surface composed of invariant and highly conserved residues from β-propeller blades;

(b) a three-sided pocket formed by Trp426, Thr386, and Arg 485 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);

(c) a three-sided pocket formed by Trp426, Thr441, Thr 465, and Arg 485 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);

(d) a hydrophobic pocket composed of Trp 426, Trp 717, Thr 386, and Val 384 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);

(e) a pocket formed by Leu634, Met590, and Tyr574 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.); and

(f) a pocket formed by Arg485, Arg467, Arg534, Tyr548, and Arg572 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);.

A binding pocket may comprise one or more of the amino acid residues for an F-box protein crystal or F-box protein –substrate crystal identified in Table 3 or Table 4. In an aspect the binding pocket comprises the atomic contacts of atomic interactions 1 to 4 or interactions 5 to 8/9 identified in Table 3 or Table 4. In an aspect of the invention the binding pocket comprises all of the amino acid residues identified in Table 3 or Table 4.

The term "binding pocket" (BP) also includes a homolog of the binding pocket or a portion thereof. As used herein, the term "homolog" in reference to a binding pocket refers to a binding pocket or a portion thereof which may have deletions, insertions or substitutions of amino acid residues as long as the binding specificity is retained. In this regard, deliberate amino acid substitutions may be made on the basis of similarity in polarity, charge, solubility, hydrophobicity, hydrophilicity, and/or the amphipathic nature of the residues as long as the binding specificity of the binding pocket is retained.

As used herein, the term "portion thereof" means the structural coordinates corresponding to a sufficient number of amino acid residues of a binding pocket (or homologs thereof) that are capable of associating with a substrate (e.g. CPD motif) or ligand. For example, the structural coordinates provided in a crystal structure may contain a subset of the amino acid residues in a binding pocket which may be useful in the modelling and design of compounds that bind to the binding pocket.

CRYSTAL

The invention provides crystal structures. As used herein, the term "crystal" or "crystalline" means a structure (such as a three dimensional (3D) solid aggregate) in which the plane faces intersect at definite angles and in which there is a regular structure (such as internal structure) of the constituent chemical species. The term "crystal" can include any one of: a solid physical crystal form such as an experimentally prepared crystal, a crystal structure derivable from the crystal (including secondary and/or tertiary and/or quaternary structural elements), a 2D and/or 3D model based on the crystal structure, a representation thereof such as a schematic representation thereof or a diagrammatic representation thereof, or a data set thereof for a computer.

In one aspect, the crystal is usable in X-ray crystallography techniques. Here, the crystals used can withstand exposure to X-ray beams used to produce a diffraction pattern data necessary to solve the X-ray crystallographic structure. A crystal may be characterized as being capable of diffracting x-rays in a pattern defined by one of the crystal forms depicted in Blundel et al 1976, Protein Crystallography, Academic Press.

A crystal of the invention is generally produced in a laboratory; that is, it is an isolated crystal produced by an individual.

The invention contemplates a crystal comprising a binding pocket of the invention, in particular a binding pocket of an F-box protein or SCF complex or portion thereof, involved in substrate selection and/or orientation.

In an aspect of the invention a crystal is provided that comprises the WD40 repeat domain of an F-box protein, in particular Cdc4. In another embodiment the crystal comprises a WD40 repeat domain and a helical linker of an F-box protein. In a further embodiment, the crystal comprises a WD40 repeat domain, a helical linker and an F-box domain of an F-box protein. In an embodiment the F-box protein is a cdc4 polypeptide or portion thereof.

A crystal of the invention comprising a WD40 repeat domain, in particular a Cdc4 polypeptide WD40 repeat domain, may be characterized by one or more of the following characteristics:

(a) a 7 or 8 blade β-propeller structure, in particular a 8 blade β-propeller structure;

(b) a disk like structure characterized by a cavity in the middle and two opposing circular surfaces of different size;

(c) a conical frustum of about 40Å top surface and about 50Å bottom surface, an overall thickness of 30Å and a central pore of 6Å diameter; and

(d) a CPD binding site on the top surface of the frustum of (c) and running across the edge of the pore, while the bottom surface of the frustum links to the F-box domain.

Each blade of the β-propeller structure can be further characterized by 4 anti-parallel β-strands. The disk like structure can also be characterized by a smaller surface comprising a CPD binding site and a bottom surface anchored by a helix (e.g. helix α6) of a helical extension of the F-box protein. As illustrated in Figures 2 and 3 the structure is further characterized by β-propeller blade 2 consisting of 5β-strands and a strand β9' forming a parallel arrangement with strand β9.

A crystal of a binding pocket of an F-box protein of the invention, in particular a Cdc4 polypeptide, may be characterized by one or more of the following characteristics:

(i) a dedicated pThr-Pro binding pocket;

(ii) a deep hydrophobic pocket that selects hydrophobic residues N-terminal to the phosphorylation site of a CPD motif, and

(iii) a through space electrostatic selection against basic residues C-terminal to the phosphorylation site of a CPD motif.

In a preferred embodiment, a crystal of a WD40 repeat domain has the structure illustrated in Figure 2 or 3.

A crystal of the invention can comprise a helical linker characterized by α helices that form a stalk and pedestal like structure that connects and orients a WD repeat domain. A helical linker structure of a Cdc4 polypeptide can also be characterized by one or more of the following structures:(a) a helix (e.g. α6 in Figure 2 or Figure 6) that is 30Å in length and is anchored at its N-terminus to the hydrophobic core of the F-box/helical extension and at its C-terminus to the hydrophobic core of a WD repeat domain,

(b) the helix of (a) (e.g. α6) anchored at its amino terminus to an F-box through hydrophobic interactions (e.g. involving α6 residues Phe 355, Leu356, and F box residues Ile295, Ile296, Leu315, and Trp316 or the corresponding residues in Cdc4 homologs, variants, precursors etc.));

(c) a second helix (e.g. helix 5) packed along the base of the helix of (a) or (b) opposite to the F-box domain through hydrophobic interactions (e.g. involving Tyr342, Leu338, and Leu 334) (or the corresponding residues in Cdc4 homologs, variants, precursors etc.) ;

(d) the helix of (a) (e.g. helix α6) anchored at its C-terminus through hydrophobic interactions;

(e) a C-terminal end of helix α6 inserted obliquely between propeller blades β7 and β8 of the WD40 domain through van der Wals and hydrophobic interactions (e.g. involving Trp365 and Ile361 with WD40 domain residues Val687, Ile696, Leu726, and Phe743 in β-propeller bnlades 7 and 8 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.).

In a preferred embodiment, a crystal of a helical linker has the structure illustrated in Figure 2.

A crystal of the invention may comprise a CPD motif binding pocket that is characterized by a hydrophobic pocket that surrounds the open central channel of a 7 or 8 blade WD repeat propeller. A crystal of a Cdc4 polypeptide may be more particularly characterized by one or more of the following:

(a) a WD repeat domain surface composed of invariant and highly conserved residues from β-propeller blades;

(b) a three-sided pocket formed by Trp426, Thr386, and Arg 485 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);

(c) a three-sided pocket formed by Trp426, Thr441, Thr 465, and Arg 485 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);

(d) a hydrophobic pocket composed of Trp 426, Trp 717, Thr 386, and Val 384(or the corresponding residues in Cdc4 homologs, variants, precursors etc.);

(e) a pocket formed by Leu634, Met590, and Tyr574 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.); and

(f) a pocket formed by Arg485, Arg467, Arg534, Tyr548, and Arg572 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.).

In a preferred embodiment, a crystal of a CPD motif binding pocket has the structure illustrated in Figure 3, 4, 6 or 7

In a further aspect of the invention a crystal is provided comprising an F-box domain comprising five α helices. In a preferred embodiment, a crystal of an F-box domain has the structure illustrated in Figure 2 or Figure 6.

A crystal of the invention may comprise an F-box protein characterized by one or more of the following:

(a) an F-box domain consisting of five α helices;

(b) a WD 40 repeat domain characterized by 7 or 8 copies of a WD40 repeat motif forming a 7 or 8 blade β-propeller structure; and

(c) two α helices that together with two α helices of the F-box domain forming a stalk and pedestal like structure that connects and orients the WD40 domain.

With reference to a crystal of the present invention, residues in a binding pocket may be defined by their spatial proximity to a substrate or ligand in the crystal structure. For example, a binding pocket may be defined by its proximity to a substrate molecule, or modulator.

A crystal of the invention includes a binding pocket in association with one or more moieties, including heavy-metal atoms i.e. a derivative crystal, or one or more substrates or ligands i.e. a co-crystal.

The term "associate", "association" or "associating" refers to a condition of proximity between a moiety (i.e. chemical entity or compound or portions or fragments thereof), and a binding pocket. The association may be non-covalent i.e. where the juxtaposition is energetically favored by for example, hydrogen-bonding, van der Waals, or electrostatic or hydrophobic interactions, or it may be covalent.

The term "heavy-metal atoms" refers to an atom that can be used to solve an x-ray crystallography phase problem, including but not limited to a transition element, a lanthanide metal, or an actinide metal. Lanthanide metals include elements with atomic numbers between 57 and 71, inclusive. Actinide metals include elements with atomic numbers between 89 and 103, inclusive.

Multiwavelength anomalous diffraction (MAD) phasing may be used to solve protein structures using selenomethionyl (SeMet) proteins. Therefore, a complex of the invention may comprise a crystalline binding pocket with selenium on the methionine residues of the protein.

A crystal may comprise a complex between a binding pocket and one or more substrates or ligands. In other words the binding pocket may be associated with one or more ligands or molecules in the crystal. The ligand may be any compound that is capable of stably and specifically associating with the binding pocket. A ligand may, for example, be a modulator or analogue thereof. Therefore, a crystal may comprise a binding pocket comprising two or more of the amino acid residues of an F-box protein structure as described herein, that are capable of associating with or coordinating a CPD motif as described herein.

In an embodiment, a crystal of the invention comprises a complex between a binding pocket, and a substrate or analogue thereof. Therefore, the present invention also provides a crystal comprising a binding pocket of an F-box protein or a SCF complex and a substrate or analogue thereof. A substrate may be for example, a CPD motif or CPD motif containing protein. An analog of a substrate is one which mimics the substrate molecule, binding in the binding pocket, but which is incapable (or has a significantly reduced capacity) to take part in SCF E3 ubiquitin ligase activity.

In an embodiment, a crystal comprising a WD repeat domain of a Cdc4 polypeptide and a CPD motif is provided, which is characterized by one or more of the following:

(a) a WD 40 repeat domain characterized by 7 or 8 copies of a WD40 repeat motif forming a 7 or 8 blade β-propeller structure comprising β-propeller blades 1, 2, 3, 4, 5, 6, and 7, and optionally 8;

(b) the CPD motif binds in an extended manner across β-propeller blade 2 with the N-terminus oriented toward the central cavity of the WD repeat domain and the C-terminus oriented towards the outer rim;

(c) the CPD binding surface of the WD repeat domain is composed of invariant and highly conserved residues from β-propeller blades 1 to 6 and optionally 8;

(d) a P0 phosphate pThr of the CPD motif forms direct electrostatic interactions with the guanidium groups of Arg 485, Arg 467, and Arg 534 and a direct hydrogen bond with the side chain of Tyr 548 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);

(e) P +1 proline side chains of the CPD motif project into a three-sided pocket on the CPD binding surface formed by the side chain of Trp 426 and Arg485 or Trp 426, Thr441, Thr465, and Arg 485 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.); and

(f) P+1 leucine side chain of the CPD motif is oriented towards a hydrophobic pocket composed of residues Trp 426, Trp 717, Thr 386, and Val 384 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.).

In a preferred embodiment, a crystal of a complex of a WD repeat domain and a CPD motif has the structure illustrated in Figure 2, 3, 4, 6, or 7.

A crystal or secondary or three-dimensional structure of a binding pocket of an F-box protein, may be specifically defined by one or more of the atomic contacts of the atomic interactions identified in Table 3 or Table 4. The atomic interactions in Table 3 or Table 4 are defined therein by an atomic contact (more preferably, a specific atom of an amino acid residue where indicated) on the F box protein, in particular on the WD40 repeat domain or helical linker, and an atomic contact (more preferably, a specific atom of an amino acid residue where indicated) on a substrate e.g. CPD motif, or an atomic contact (more preferably, a specific atom of an amino acid residue where indicated) on another region of the F-box protein (e.g. helical linker or F-box domain). In certain embodiments, a crystal of the invention comprises the atomic contacts of atomic interactions 1 to 8 identified in Table 3 or Table 4. In certain particular embodiments a crystal is provided comprising the atomic contacts of atomic interactions 1 to 4 or 5 to 8. Preferably, a crystal is defined by the atoms of the atomic contacts in the binding pocket having the structural coordinates for the atoms listed in Table 6.

A structure of a complex may be defined by selected intermolecular contacts, preferably the structural coordinates of the intermolecular contacts as defined in Table 6, preferably interactions 5 to 8.

A crystal of the invention may comprise one or more of the following groups of amino acid residues: (a) Ile 295, Ile 296, Leu 315, Trp 316, Leu 319, Phe 355, and Leu 356; (b) Val 687, Ile 696, Leu 726, Phe 743, Trp 365, and

Ile 364; (c) Asn 684, Arg 700, and Glu 323; (d) Arg 485, Arg 467, Arg 534, Tyr 548; (e) Trp 426, Arg 485, Thr 441, and Thr 465; (f) Trp 426, Trp 717, Thr 386, and Val 384; (g) Tyr 574, Thr 386 and Val 384; (h) Tyr 574, Met 590, and Leo 634; and (i) the corresponding residues in Cdc4 homologs, paralogs, variants, or precursors. Preferably the atoms of the amino acid residues have the structural coordinates as set out in Table 6.

A crystal of the invention may enable the determination of structural data for a substrate or ligand. In order to be able to derive structural data for a ligand, or substrate it is necessary for the molecule to have sufficiently strong electron density to enable a model of the molecule to be built using standard techniques. For example, there should be sufficient electron density to allow a model to be built using XTALVIEW (McRee 1992 J. Mol. Graphics. 10 44-46).

A crystal of the invention may belong to space group $P3_2$. The term "space group" refers to the lattice and symmetry of the crystal. In a space group designation the capital letter indicates the lattice type and the other symbols represent symmetry operations that can be carried out on the contents of the asymmetric unit without changing its appearance.

A crystal of the invention may comprise a unit cell having the following unit dimensions: a =107.7Å, b = 107.7Å, c = 168.3Å, $\alpha = \gamma = 90°$, β =120°. The term "unit cell" refers to the smallest and simplest volume element (i.e. parallelpiped-shaped block) of a crystal that is completely representative of the unit of pattern of the crystal. The unit cell axial lengths are represented by a, b, and c. Those of skill in the art understand that a set of atomic coordinates determined by X-ray crystallography is not without standard error.

In a preferred embodiment, a crystal of the invention has the structural coordinates as shown in Table 6. As used herein, the term "structural coordinates" refers to a set of values that define the position of one or more amino acid residues with reference to a system of axes. The term refers to a data set that defines the three dimensional structure of a molecule or molecules (e.g. Cartesian coordinates, temperature factors, and occupancies). Structural coordinates can be slightly modified and still render nearly identical three dimensional structures. A measure of a unique set of structural coordinates is the root-mean-square deviation of the resulting structure. Structural coordinates that render three dimensional structures (in particular a three dimensional structure of a ligand binding pocket) that deviate from one another by a root-mean-square deviation of less than 5 Å, 4 Å, 3 Å, 2 Å, 1.5 Å. 1.0 Å, or 0.5 Å may be viewed by a person of ordinary skill in the art as very similar.

Variations in structural coordinates may be generated because of mathematical manipulations of the structural coordinates of a structure or binding pocket described herein. For example, the structural coordinates of Table 6 may be manipulated by crystallographic permutations of the structural coordinates, fractionalization of the structural coordinates, integer additions or substractions to sets of the structural coordinates, inversion of the structural coordinates or any combination of the above.

Variations in the crystal structure due to mutations, additions, substitutions, and/or deletions of the amino acids, or other changes in any of the components that make up the crystal may also account for modifications in structural coordinates. If such modifications are within an acceptable standard error as compared to the original structural coordinates, the resulting structure may be the same. Therefore, a ligand that bound to a binding pocket of

an F-box protein, would also be expected to bind to another binding pocket whose structural coordinates defined a shape that fell within the acceptable error. Such modified structures of a binding pocket thereof are also within the scope of the invention.

Various computational analyses may be used to determine whether a molecule or the binding pocket thereof is sufficiently similar to all or parts of an F-box or a binding pocket thereof. Such analyses may be carried out using conventional software applications and methods as described herein.

A crystal of the invention may also be specifically characterised by the parameters, diffraction statistics and/or refinement statistics set out in Table 1 or in Table 2.

Illustrations of particular crystals of the invention are shown in Figures 2, 3, 4, 6 and 7.

METHOD OF MAKING A CRYSTAL

The present invention also provides a method of making a crystal according to the invention. The crystal may be formed from an aqueous solution comprising a purified polypeptide comprising an F-box protein including a variant, part, homolog, or fragment thereof (e.g. a binding pocket). A method may utilize a purified polypeptide comprising a binding pocket to form a crystal. A method may utilize one or more purified mutant polypeptides as described herein. In an embodiment, a mutant cdc4 polypeptide is used to make crystals.

The term "purified" in reference to a polypeptide, does not require absolute purity such as a homogenous preparation rather it represents an indication that the polypeptide is relatively purer than in the natural environment. Generally, a purified polypeptide is substantially free of other proteins, lipids, carbohydrates, or other materials with which it is naturally associated, preferably at a functionally significant level for example at least 85% pure, more preferably at least 95% pure, most preferably at least 99% pure. A skilled artisan can purify a polypeptide comprising using standard techniques for protein purification. A substantially pure polypeptide will yield a single major band on a non-reducing polyacrylamide gel. Purity of the polypeptide can also be determined by amino-terminal amino acid sequence analysis.

A polypeptide used in the method may be chemically synthesized in whole or in part using techniques that are well-known in the art. Alternatively, methods are well known to the skilled artisan to construct expression vectors containing a native or mutated protein coding sequence and appropriate transcriptional/translational control signals. These methods include *in vitro* recombinant DNA techniques, synthetic techniques, and *in vivo* recombination/genetic recombination. See for example the techniques described in Sambrook et al. (Molecular Cloning: A Laboratory Manual, 2nd Edition, Cold Spring Harbor Laboratory press (1989)), and other laboratory textbooks. (See also Sarker et al, Glycoconjugate J. 7:380, 1990; Sarker et al, Proc. Natl. Acad, Sci. USA 88:234-238, 1991, Sarker et al, Glycoconjugate J. 11: 204-209, 1994; Hull et al, Biochem Biophys Res Commun 176:608, 1991 and Pownall et al, Genomics 12:699-704, 1992).

Crystals may be grown from an aqueous solution containing the purified polypeptide by a variety of conventional processes. These processes include batch, liquid, bridge, dialysis, vapor diffusion, and hanging drop methods. (See for example, McPherson, 1982 John Wiley, New York; McPherson, 1990, Eur. J. Biochem. 189: 1-23;

Webber. 1991, Adv. Protein Chem. 41:1-36). Generally, native crystals of the invention are grown by adding precipitants to the concentrated solution of the polypeptide. The precipitants are added at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

Derivative crystals of the invention can be obtained by soaking native crystals in a solution containing salts of heavy metal atoms. A complex of the invention can be obtained by soaking a native crystal in a solution containing a compound that binds the polypeptide, or they can be obtained by co-crystallizing the polypeptide in the presence of one or more compounds. In order to obtain co-crystals with a compound which binds deep within the tertiary structure of the polypeptide it is necessary to use the second method.

Once the crystal is grown it can be placed in a glass capillary tube and mounted onto a holding device connected to an X-ray generator and an X-ray detection device. Collection of X-ray diffraction patterns are well documented by those skilled in the art (See for example, Ducruix and Geige, 1992, IRL Press, Oxford, England). A beam of X-rays enter the crystal and diffract from the crystal. An X-ray detection device can be utilized to record the diffraction patterns emanating from the crystal. Suitable devices include the Marr 345 imaging plate detector system with an RU200 rotating anode generator.

Multiwavelength anomalous diffraction (MAD) phasing using selenomethionyl (SeMet) proteins may be used to determine a crystal of the invention. Thus, the invention contemplates a method for determining a crystal structure of the invention using a selenomethionyl derivative of an F-box protein or SCF complex, including a variant, part, homolog or fragement thereof.

Methods for obtaining the three dimensional structure of the crystalline form of a molecule or complex are described herein and known to those skilled in the art (see Ducruix and Geige 1992, IRL Press, Oxford, England). Generally, the x-ray crystal structure is given by the diffraction patterns. Each diffraction pattern reflection is characterized as a vector and the data collected at this stage determines the amplitude of each vector. The phases of the vectors may be determined by the isomorphous replacement method where heavy atoms soaked into the crystal are used as reference points in the X-ray analysis (see for example, Otwinowski, 1991, Daresbury, United Kingdom, 80-86). The phases of the vectors may also be determined by molecular replacement (see for example, Naraza, 1994, Proteins 11:281-296). The amplitudes and phases of vectors from the crystalline form determined in accordance with these methods can be used to analyze other related crystalline polypeptides.

The unit cell dimensions and symmetry, and vector amplitude and phase information can be used in a Fourier transform function to calculate the electron density in the unit cell i.e. to generate an experimental electron density map. This may be accomplished using the PHASES package (Furey, 1990). Amino acid sequence structures are fit to the experimental electron density map (i.e. model building) using computer programs (e.g. Jones, TA. et al, Acta Crystallogr A47, 100-119, 1991). This structure can also be used to calculate a theoretical electron density map. The theoretical and experimental electron density maps can be compared and the agreement between the maps can be described by a parameter referred to as R-factor. A high degree of overlap in the maps is represented by a low value

R-factor. The R-factor can be minimized by using computer programs that refine the structure to achieve agreement between the theoretical and observed electron density map. For example, the XPLOR program, developed by Brunger (1992, Nature 355:472-475) can be used for model refinement.

A three dimensional structure of the molecule or complex may be described by atoms that fit the theoretical electron density characterized by a minimum R value. Files can be created for the structure that defines each atom by coordinates in three dimensions.

MUTANT CDC4 POLYPEPTIDES

The present invention provides novel mutant cdc4 polypeptides.

A particular mutant of the present invention is a polypeptide having an amino acid sequence of a cdc4 polypeptide wherein amino acid residues are replaced or deleted providing a cdc4 polypeptide that can be produced by recombinant techniques and retains its activity, for example its ability to associate with a CPD motif.

In an aspect a cdc4 sequence is mutated by deleting the region from the beginning of the F-box domain to the end of the WD40 repeat domain. In particular, terminal residues 1 to 262 and 745 to 779 can be deleted from the cdc4 seqeunce.

Other additions, substitutions, and/or deletions may be made to the cdc4 mutants of the present invention. In an embodiment cdc4 can be engineered to remove flexible loops comprising residues 601 to 604 and 609 to 624.

Particular mutant cdc4 polypeptides of the invention are also identified in Table 5.

The present invention also relates to nucleic acid molecules or polynucleotides encoding a cdc4 mutant polypeptide. The polynucleotides can be used to transform host cells to express the cdc4 mutant polypeptides of the invention. They can also be used as a probe to detect related enzymes.

The present invention still further relates to recombinant vectors that include the nucleic acid molecules of the invention. The nucleic acid molecules of the invention may be inserted into an appropriate vector, and the vector may contain the necessary elements for the transcription and translation of an inserted coding sequence. Accordingly, vectors may be constructed which comprise a nucleic acid molecule of the invention, and where appropriate one or more transcription and translation elements linked to the nucleic acid molecule. A vector can be used to transform host cells. Therefore, the invention provides host cells containing a vector of the invention. As well, the invention provides methods of making such vectors and host cells.

The mutant cdc4 polypeptides of the invention can be encoded, expressed, and purified by any one of a number of methods known to those skilled in the art. Preferred production methods will depend on many factors including the costs and availability of materials and other economic considerations. The optimum production procedure for a given situation will be apparent to those skilled in the art through minimal experimentation.

In accordance with an aspect of the present invention, there is provided a process for producing a cdc4 mutant polypeptide by recombinant techniques utilizing the nucleic acid molecules of the invention. The method may comprise culturing recombinant host cells containing a nucleic acid sequence encoding a cdc4 mutant polypeptide,

under conditions promoting expression of the cdc4 mutant polypeptide, and subsequent recovery of the cdc4 mutant polypeptide.

The invention further broadly contemplates a recombinant cdc4 mutant polypeptide obtained using a method of the invention.

A cdc4 mutant polypeptide of the invention may be conjugated with other molecules, such as polypeptides, to prepare fusion polypeptides or chimeric polypeptides. This may be accomplished, for example, by the synthesis of N-terminal or C-terminal fusion polypeptides.

The invention further contemplates antibodies having specificity against a cdc4 mutant polypeptide of the invention. Antibodies may be labeled with a detectable substance and used to detect cdc4 mutant polypeptides. In another embodiment, the invention provides an isolated antibody that binds specifically to a cdc4 mutant polypeptide.

The cdc4 mutant polypeptides of the present invention are particularly well suited for use in screening methods for identifying modulators of cdc4 or SCF complexes.

Still further the invention provides a method for evaluating a test compound for its ability to modulate the biological activity of a cdc4 polypepide. In this application, "modulate" refers to a change or an alteration in the biological activity of a cdc4 polypeptide. Modulation may be an increase or a decrease in activity, a change in characteristics (e.g. kinetic characteristics), or any other change in the biological, functional, or immunological properties of the polypeptide.

The substances and compounds identified using the methods of the invention, may be used to modulate the biological activity of a cdc4 polypeptide or a SCF complex, and they may be used in the treatment of conditions mediated by a cdc4 polypeptide or SCF complex. Accordingly, the substances and compounds may be formulated into compositions for administration to individuals suffering from one or more of these conditions. Therefore, the present invention also relates to a composition comprising one or more of a substance or compound identified using a method of the invention, and a pharmaceutically acceptable carrier, excipient or diluent. A method for treating or preventing these conditions is also provided comprising administering to a patient in need thereof, a composition of the invention.

MODEL

A crystal structure of the present invention may be used to make a model of a binding pocket of a SCF E3 ubiquitin ligase, in particular an F-box protein, that is involved in substrate selection and/or orientation. A model may, for example, be a structural model or a computer model. A model may represent the secondary, tertiary and/or quaternary structure of the binding pocket. The model itself may be in two or three dimensions. It is possible for a computer model to be in three dimensions despite the constraints imposed by a conventional computer screen, if it is possible to scroll along at least a pair of axes, causing "rotation" of the image.

As used herein, the term "modelling" includes the quantitative and qualitative analysis of molecular structure and/or function based on atomic structural information and interaction models. The term "modelling" includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry and other structure-based constraint models.

Preferably, modelling is performed using a computer and may be further optimized using known methods. This is called modelling optimisation.

An integral step to an approach of the invention for designing modulators (e.g. inhibitors) of a subject F-box protein or SCF complex involves construction of computer graphics models of a binding pocket of the invention which can be used to design pharmacophores by rational drug design. For instance, for an inhibitor to interact optimally with the subject binding pocket, it will generally be desirable that it have a shape which is at least partly complimentary to that of a particular binding pocket of the protein, as for example those binding pockets of the protein which are involved in recognition of a ligand (e.g. substrate). Additionally, other factors, including electrostatic interactions, hydrogen bonding, hydrophobic interactions, desolvation effects, and cooperative motions of ligand and receptor, all influence the binding effect and should be taken into account in attempts to design bioactive modulators (e.g. inhibitors).

As described herein, a computer-generated molecular model of the subject binding pockets can be created. In preferred embodiments, at least the Cα-carbon positions of the binding pockets are mapped to a particular coordinate pattern, such as the coordinates for a binding pocket in Table 6, by homology modeling, and the structure of the protein and velocities of each atom are calculated at a simulation temperature (T_o) at which the docking simulation is to be determined. Typically, such a protocol involves primarily the prediction of side-chain conformations in the modeled binding pocket, while assuming a main-chain trace taken from a tertiary structure such as provided in Table 6 and the Figures. Computer programs for performing energy minimization routines are commonly used to generate molecular models. For example, both the CHARMM (Brooks et al. (1983) *J Comput Chem* 4:187-217) and AMBER (Weiner et al (1981) *J. Comput. Chem.* 106: 765) algorithms handle all of the molecular system setup, force field calculation, and analysis (see also, Eisenfield et al. (1991) *Am J Physiol* 261:C376-386; Lybrand (1991) *J Pharm Belg* 46:49-54; Froimowitz (1990) *Biotechniques* 8:640-644; Burbam et al. (1990) *Proteins* 7:99-111; Pedersen (1985) *Environ Health Perspect* 61:185-190; and Kini et al. (1991) *J Biomol Struct Dyn* 9:475-488). At the heart of these programs is a set of subroutines that, given the position of every atom in the model, calculate the total potential energy of the system and the force on each atom. These programs may utilize a starting set of atomic coordinates, such as the coordinates provided in Table 6, the parameters for the various terms of the potential energy function, and a description of the molecular topology (the covalent structure). Common features of such molecular modeling methods include: provisions for handling hydrogen bonds and other constraint forces; the use of periodic boundary conditions; and provisions for occasionally adjusting positions, velocities, or other parameters in order to maintain or change temperature, pressure, volume, forces of constraint, or other externally controlled conditions.

Most conventional energy minimization methods use the input data described above and the fact that the potential energy function is an explicit, differentiable function of Cartesian coordinates, to calculate the potential energy and its gradient (which gives the force on each atom) for any set of atomic positions. This information can be used to generate a new set of coordinates in an effort to reduce the total potential energy and, by repeating this process

over and over, to optimize the molecular structure under a given set of external conditions. These energy minimization methods are routinely applied to molecules similar to the subject proteins as well as nucleic acids, polymers and zeolites.

In general, energy minimization methods can be carried out for a given temperature, T_i, which may be different than the docking simulation temperature, T_o. Upon energy minimization of the molecule at T_i, coordinates and velocities of all the atoms in the system are computed. Additionally, the normal modes of the system are calculated. It will be appreciated by those skilled in the art that each normal mode is a collective, periodic motion, with all parts of the system moving in phase with each other, and that the motion of the molecule is the superposition of all normal modes. For a given temperature, the mean square amplitude of motion in a particular mode is inversely proportional to the effective force constant for that mode, so that the motion of the molecule will often be dominated by the low frequency vibrations.

After the molecular model has been energy minimized at T_i, the system is "heated" or "cooled" to the simulation temperature, T_o, by carrying out an equilibration run where the velocities of the atoms are scaled in a step-wise manner until the desired temperature, T_o, is reached. The system is further equilibrated for a specified period of time until certain properties of the system, such as average kinetic energy, remain constant. The coordinates and velocities of each atom are then obtained from the equilibrated system.

Further energy minimization routines can also be carried out. For example, a second class of methods involves calculating approximate solutions to the constrained EOM for the protein. These methods use an iterative approach to solve for the Lagrange multipliers and, typically, only need a few iterations if the corrections required are small. The most popular method of this type, SHAKE (Ryckaert et al. (1977) *J Comput Phys* 23:327; and Van Gunsteren et al. (1977) *Mol Phys* 34:1311) is easy to implement and scales as O(N) as the number of constraints increases. Therefore, the method is applicable to macromolecules such as F-box proteins. An alternative method, RATTLE (Anderson (1983) *J Comput Phys* 52:24) is based on the velocity version of the Verlet algorithm. Like SHAKE, RATTLE is an iterative algorithm and can be used to energy minimize the model of the subject protein.

Overlays and super positioning with a three dimensional model of a binding pocket of the invention may be used for modelling optimisation. Additionally alignment and/or modelling can be used as a guide for the placement of mutations on a binding pocket to characterize the nature of the site in the context of a cell.

The three dimensional structure of a new crystal may be modelled using molecular replacement. The term "molecular replacement" refers to a method that involves generating a preliminary model of a molecule or complex whose structural coordinates are unknown, by orienting and positioning a molecule whose structural coordinates are known within the unit cell of the unknown crystal, so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in turn, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal. Lattman, E., "Use of

the Rotation and Translation Functions", in Methods in Enzymology, 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York, (1972).

Commonly used computer software packages for molecular replacement are X-PLOR (Brunger 1992, Nature 355: 472-475), AMoRE (Navaza, 1994, Acta Crystallogr. A50:157-163), the CCP4 package (Collaborative Computational Project, Number 4, "The CCP4 Suite: Programs for Protein Crystallography", Acta Cryst., Vol. D50, pp. 760-763, 1994), the MERLOT package (P.M.D. Fitzgerald, J. Appl. Cryst., Vol. 21, pp. 273-278, 1988) and XTALVIEW (McCree et al (1992) J. Mol. Graphics 10: 44-46. It is preferable that the resulting structure not exhibit a root-mean-square deviation of more than 3 Å.

Molecular replacement computer programs generally involve the following steps: (1) determining the number of molecules in the unit cell and defining the angles between them (self rotation function); (2) rotating the known structure against diffraction data to define the orientation of the molecules in the unit cell (rotation function); (3) translating the known structure in three dimensions to correctly position the molecules in the unit cell (translation function); (4) determining the phases of the X-ray diffraction data and calculating an R-factor calculated from the reference data set and from the new data wherein an R-factor between 30-50% indicates that the orientations of the atoms in the unit cell have been reasonably determined by the method; and (5) optionally, decreasing the R-factor to about 20% by refining the new electron density map using iterative refinement techniques known to those skilled in the art (refinement).

The quality of the model may be analysed using a program such as PROCHECK or 3D-Profiler [Laskowski et al 1993 J. Appl. Cryst. 26:283-291; Luthy R. et al, Nature 356: 83-85, 1992; and Bowie, J.U. et al, Science 253: 164-170, 1991]. Once any irregularities have been resolved, the entire structure may be further refined.

Other molecular modelling techniques may also be employed in accordance with this invention. See, e.g., Cohen, N. C. *et al*, "Molecular Modelling Software and Methods for Medicinal Chemistry", J. Med. Chem., 33, pp. 883-894 (1990). See also, Navia, M. A. and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

Using the structural coordinates of crystal provided by the invention, molecular modelling may be used to determine the structural coordinates of a crystalline mutant or homolog of a SCF complex or F-box binding pocket involved in substrate selection and/or orientation. By the same token a crystal of the invention can be used to provide a model of a substrate or ligand. Modelling techniques can then be used to approximate the three dimensional structure of substrate or ligand derivatives and other components which may be able to mimic the atomic contacts between a substrate or ligand and binding pocket.

COMPUTER FORMAT OF CRYSTALS/MODELS

Information derivable from a crystal of the present invention (for example the structural coordinates) and/or the model of the present invention may be provided in a computer-readable format.

Therefore, the invention provides a computer readable medium or a machine readable storage medium which comprises the structural coordinates of a binding pocket of an SCF complex of F box protein described herein

including all or any parts thereof, or substrates or ligands including portions thereof. Such storage medium or storage medium encoded with these data are capable of displaying on a computer screen or similar viewing device, a three-dimensional graphical representation of a molecule or molecular complex which comprises such binding pockets or similarly shaped homologous binding pockets. Thus, the invention also provides computerized representations of the secondary or three-dimensional structures of a binding pocket of the invention, including any electronic, magnetic, or electromagnetic storage forms of the data needed to define the structures such that the data will be computer readable for purposes of display and/or manipulation.

In an aspect the invention provides a computer for producing a three-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex comprises a binding pocket defined by structural coordinates of a binding pocket or structural coordinates of atoms of a substrate or ligand, or a three-dimensional representation of a homolog of said molecule or molecular complex, wherein said homolog comprises a binding pocket, or substrate or ligand that has a root mean square deviation from the backbone atoms not more than 1.5 angstroms wherein said computer comprises:

(a) a machine-readable data storage medium comprising a data storage material encoded with machine readable data wherein said data comprises the structural coordinates of a binding pocket or a substrate according to Table 6;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine readable data into said three-dimensional representation; and

(d) a display coupled to said central-processing unit for displaying said three-dimensional representation.

The invention also provides a computer for determining at least a portion of the structural coordinates corresponding to an X-ray diffraction pattern of a molecule or molecular complex wherein said computer comprises:

(a) a machine-readable data storage medium comprising a data storage material encoded with machine readable data wherein said data comprises the structural coordinates according to Table 6;

(b) a machine-readable data storage medium comprising a data storage material encoded with machine readable data wherein said data comprises an X-ray diffraction pattern of said molecule or molecular complex;

(c) a working memory for storing instructions for processing said machine-readable data of (a) and (b);

(d) a central-processing unit coupled to said working memory and to said machine-readable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structural coordinates; and

(e) a display coupled to said central-processing unit for displaying said structural coordinates of said molecule or molecular complex.

STRUCTURAL STUDIES

The present invention also provides a method for determining the secondary and/or tertiary structures of a polypeptide or part or complexes thereof by using a crystal, or a model according to the present invention. The polypeptide or part thereof may be any polypeptide or part thereof for which the secondary and or tertiary structure is uncharacterised or incompletely characterised. In a preferred embodiment the polypeptide shares (or is predicted to share) some structural or functional homology to a crystal of the present invention. For example, the polypeptide may show a degree of structural homology over some or all parts of the primary amino acid sequence.

The polypeptide may be an F-box protein, or part thereof with a different specificity for a substrate. Alternatively (or in addition) the polypeptide may be an F-box protein from a different species.

The polypeptide may be a mutant of a wild-type F-box protein. A mutant may arise naturally, or may be made artificially (for example using molecular biology techniques). The mutant may also not be "made" at all in the conventional sense, but merely tested theoretically using the model of the present invention. A mutant may or may not be functional.

Thus, using a model of the present invention, the effect of a particular mutation on the overall two and/or three dimensional structure of an F-box protein or SCF complex or the interaction between a binding pocket of an F-box protein or SCF complex and a substrate or ligand can be investigated.

Alternatively, the polypeptide may perform an analogous function or be suspected to show a similar mechanism to an F-box protein.

The polypeptide may also be the same as the polypeptide of the crystal, but in association with a different substrate or ligand (for example, modulator or inhibitor) or cofactor. In this way it is possible to investigate the effect of altering the substrate or ligand with which the polypeptide is associated on the structure of the binding pocket.

Secondary or tertiary structure may be determined by applying the structural coordinates of a crystal or model of the present invention to other data such as an amino acid sequence, X-ray crystallographic diffraction data, or nuclear magnetic resonance (NMR) data. Homology modeling, molecular replacement, and nuclear magnetic resonance methods using these other data sets are described below.

Homology modeling (also known as comparative modeling or knowledge-based modeling) methods develop a three dimensional model from a polypeptide sequence based on the structures of known proteins (i.e. an F-box structure or complex thereof described herein). The method utilizes a computer model of a crystal of the present invention (the "known structure"), a computer representation of the amino acid sequence of the polypeptide with an unknown structure, and standard computer representations of the structures of amino acids. The method in particular comprises the steps of; (a) identifying structurally conserved and variable regions in the known structure; (b) aligning the amino acid sequences of the known structure and unknown structure (c) generating co-ordinates of main chain atoms and side chain atoms in structurally conserved and variable regions of the unknown structure based on the coordinates of the known structure thereby obtaining a homology model; and (d) refining the homology model to obtain a three dimensional structure for the unknown structure. This method is well known to those skilled in the art

(Greer, 1985, Science 228, 1055; Bundell et al 1988, Eur. J. Biochem. 172, 513; Knighton et al., 1992, Science 258:130-135, http://biochem.vt.edu/courses/modeling/ homology.htn). Computer programs that can be used in homology modelling are Quanta and the Homology module in the Insight II modelling package distributed by Molecular Simulations Inc, or MODELLER (Rockefeller University, www.iucr.ac.uk/sinris-top/logical/prg-modeller.html).

In step (a) of the homology modelling method, a known structure is examined to identify the structurally conserved regions (SCRs) from which an average structure, or framework, can be constructed for these regions of the protein. Variable regions (VRs), in which known structures may differ in conformation, also must be identified. SCRs generally correspond to the elements of secondary structure, such as alpha-helices and beta-sheets, and to ligand- and substrate-binding sites. The VRs usually lie on the surface of the proteins and form the loops where the main chain turns.

Many methods are available for sequence alignment of known structures and unknown structures. Sequence alignments generally are based on the dynamic programming algorithm of Needleman and Wunsch [J. Mol. Biol. 48: 442-453, 1970]. Current methods include FASTA, Smith-Waterman, and BLASTP, with the BLASTP method differing from the other two in not allowing gaps. Scoring of alignments typically involves construction of a 20x20 matrix in which identical amino acids and those of similar character (i.e., conservative substitutions) may be scored higher than those of different character. Substitution schemes which may be used to score alignments include the scoring matrices PAM (Dayhoff et al., Meth. Enzymol. 91: 524-545, 1983), and BLOSUM (Henikoff and Henikoff, Proc. Nat. Acad. Sci. USA 89: 10915-`0919, 1992), and the matrices based on alignments derived from three-dimensional structures including that of Johnson and Overington (JO matrices) (J. Mol. Biol. 233: 716-738, 1993).

Alignment based solely on sequence may be used; however, other structural features also may be taken into account. In Quanta, multiple sequence alignment algorithms are available that may be used when aligning a sequence of the unknown with the known structures. Four scoring systems (i.e. sequence homology, secondary structure homology, residue accessibility homology, CA-CA distance homology) are available, each of which may be evaluated during an alignment so that relative statistical weights may be assigned.

When generating coordinates for the unknown structure, main chain atoms and side chain atoms, both in SCRs and VRs need to be modelled. A variety of approaches known to those skilled in the art may be used to assign co-ordinates to the unknown. In particular, the co-ordinates of the main chain atoms of SCRs will be transferred to the unknown structure. VRs correspond most often to the loops on the surface of the polypeptide and if a loop in the known structure is a good model for the unknown, then the main chain co-ordinates of the known structure may be copied. Side chain coordinates of SCRs and VRs are copied if the residue type in the unknown is identical to or very similar to that in the known structure. For other side chain coordinates, a side chain rotamer library may be used to define the side chain coordinates. When a good model for a loop cannot be found fragment databases may be searched for loops in other proteins that may provide a suitable model for the unknown. If desired, the loop may then be subjected to conformational searching to identify low energy conformers if desired.

Once a homology model has been generated it is analyzed to determine its correctness. A computer program available to assist in this analysis is the Protein Health module in Quanta which provides a variety of tests. Other programs that provide structure analysis along with output include PROCHECK and 3D-Profiler [Luthy R. et al, Nature 356: 83-85, 1992; and Bowie, J.U. et al, Science 253: 164-170, 1991]. Once any irregularities have been resolved, the entire structure may be further refined. Refinement may consist of energy minimization with restraints, especially for the SCRs. Restraints may be gradually removed for subsequent minimizations. Molecular dynamics may also be applied in conjunction with energy minimization.

Molecular replacement involves applying a known structure to solve the X-ray crystallographic data set of a polypeptide of unknown structure. The method can be used to define the phases describing the X-ray diffraction data of a polypeptide of unknown structure when only the amplitudes are known. Thus in an embodiment of the invention, a method is provided for determining three dimensional structures of polypeptides with unknown structure by applying the structural coordinates of a crystal of the present invention to provide an X-ray crystallographic data set for a polypeptide of unknown structure, and (b) determining a low energy conformation of the resulting structure.

The structural coordinates of a crystal of the present invention may be applied to nuclear magnetic resonance (NMR) data to determine the three dimensional structures of polypeptides with uncharacterised or incompletely characterised sturcture. (See for example, Wuthrich, 1986, John Wiley and Sons, New York: 176-199; Pflugrath et al., 1986, J. Molecular Biology 189: 383-386; Kline et al., 1986 J. Molecular Biology 189:377-382). While the secondary structure of a polypeptide may often be determined by NMR data, the spatial connections between individual pieces of secondary structure are not as readily determined. The structural coordinates of a polypeptide defined by X-ray crystallography can guide the NMR spectroscopist to an understanding of the spatial interactions between secondary structural elements in a polypeptide of related structure. Information on spatial interactions between secondary structural elements can greatly simplify Nuclear Overhauser Effect (NOE) data from two-dimensional NMR experiments. In addition, applying the structural coordinates after the determination of secondary structure by NMR techniques simplifies the assignment of NOE's relating to particular amino acids in the polypeptide sequence and does not greatly bias the NMR analysis of polypeptide structure.

In an embodiment, the invention relates to a method of determining three dimensional structures of polypeptides with unknown structures, by applying the structural coordinates of a crystal of the present invention to nuclear magnetic resonance (NMR) data of the unknown structure. This method comprises the steps of: (a) determining the secondary structure of an unknown structure using NMR data; and (b) simplifying the assignment of through-space interactions of amino acids. The term " through-space interactions" defines the orientation of the secondary structural elements in the three dimensional structure and the distances between amino acids from different portions of the amino acid sequence. The term "assignment" defines a method of analyzing NMR data and identifying which amino acids give rise to signals in the NMR spectrum.

SCREENING METHODS

Another aspect of the present invention is the design and identification of agents that inhibit or potentiate an interaction between an F-box protein or an SCF E3 ubiquitin ligase and a substrate. The rationale design and identification of agents can be accomplished by utilizing the structural coordinates that define a binding pocket of the present invention involved in substrate selection and/or orientation.

The structures described herein, and the structures of other polypeptides determined by homology modeling, molecular replacement, and NMR techniques described herein can also be applied to modulator design and identification methods.

The invention contemplates molecular models, in particular three-dimensional molecular models of binding pockets of the present invention involved in substrate selection and/or orientation, and their use as templates for the design of agents able to mimic or inhibit substrate binding (e.g. modulators).

In certain embodiments, the present invention provides a method of screening for a ligand that associates with a binding pocket and/or modulates the function of a F-box protein or SCF complex by using a crystal or a model according to the present invention. The method may involve investigating whether a test compound is capable of associating with or binding a binding pocket, and/or inhibiting or enhancing interactions of atomic contacts in a binding pocket.

In accordance with an aspect of the present invention, a method is provided for screening for a ligand capable of binding to a binding pocket, wherein the method comprises using a crystal or model according to the invention.

In another aspect, the invention relates to a method of screening for a ligand capable of binding to a binding pocket, wherein the binding pocket is defined by the structural coordinates given herein, the method comprising contacting the binding pocket with a test compound and determining if the test compound binds to the binding pocket.

In one embodiment, the present invention provides a method of screening for a test compound capable of interacting with one or more key amino acid residues of a binding pocket of the present invention. For example, a test compound that interacts with one or more of amino acids of a binding pocket may prevent interaction of the F-box protein or complex thereof and its substrate resulting in modification of the SCF E3 ubiquitin ligase activity.

Another aspect of the invention provides a process comprising the steps of:

(a) performing a method of screening for a ligand described above;

(b) identifying one or more ligands capable of binding to a binding pocket; and

(c) preparing a quantity of said one or more ligands.

A further aspect of the invention provides a process comprising the steps of;

(a) performing a method of screening for a ligand as described above;

(b) identifying one or more ligands capable of binding to a binding pocket; and

(c) preparing a pharmaceutical composition comprising said one or more ligands.

Once a test compound capable of interacting with one or more key amino acid residues in a binding pocket of the present invention has been identified, further steps may be carried out either to select and/or modify compounds

and/or to modify existing compounds, to modulate the interaction with the key amino acid residues in the binding pocket.

Yet another aspect of the invention provides a process comprising the steps of;

(a) performing the method of screening for a ligand as described above;

(b) identifying one or more ligands capable of binding to a binding pocket;

(c) modifying said one or more ligands capable of binding to a binding pocket;

(d) performing said method of screening for a ligand as described above; and

(e) optionally preparing a pharmaceutical composition comprising said one or more ligands.

In another aspect of the invention, a method of screening for a test compound is provided comprising screening for test compounds that affect (inhibit or potentiate) an interaction between an F-box protein or SCF complex and a substrate as defined by interactions 1 to 4 or 5 to 8/9 in Table 3 or Table 4.

As used herein, the term "test compound" means any compound which is potentially capable of associating with a binding pocket, inhibiting or enhancing interactions of atomic contacts in a binding pocket. If, after testing, it is determined that the test compound does bind to the binding pocket, inhibits or enhances interactions of atomic contacts in a binding pocket, it is known as a "ligand".

The test compound may be designed or obtained from a library of compounds which may comprise peptides, as well as other compounds, such as small organic molecules and particularly new lead compounds. By way of example, the test compound may be a natural substance, a biological macromolecule, or an extract made from biological materials such as bacteria, fungi, or animal (particularly mammalian) cells or tissues, an organic or an inorganic molecule, a synthetic test compound, a semi-synthetic test compound, a carbohydrate, a monosaccharide, an oligosaccharide or polysaccharide, a glycolipid, a glycopeptide, a saponin, a heterocyclic compound, a structural or functional mimetic, a peptide, a peptidomimetic, a derivatised test compound, a peptide cleaved from a whole protein, or a peptide synthesised synthetically (such as, by way of example, either using a peptide synthesizer or by recombinant techniques or combinations thereof), a recombinant test compound, a natural or a non-natural test compound, a fusion protein or equivalent thereof and mutants, derivatives or combinations thereof.

The increasing availability of biomacromolecule structures of potential pharmacophoric molecules that have been solved crystallographically has prompted the development of a variety of direct computational methods for molecular design, in which the steric and electronic properties of substrate binding sites are use to guide the design of potential ligands (Cohen et al. (1990) *J. Med. Cam.* 33: 883-894; Kuntz et al. (1982) *J. Mol. Biol* 161: 269-288; DesJarlais (1988) *J. Med. Cam.* 31: 722-729; Bartlett et al. (1989) (*Spec. Publ., Roy. Soc. Chem.*) 78: 182-196; Goodford et al. (1985) *J. Med. Cam.* 28: 849-857; DesJarlais et al. *J. Med. Cam.* 29: 2149-2153). Directed methods generally fall into two categories: (1) design by analogy in which 3-D structures of known molecules (such as from a crystallographic database) are docked to the structure and scored for goodness-of-fit; and (2) *de novo* design, in which the ligand model is constructed piece-wise. The latter approach, in particular, can facilitate the development of novel molecules, uniquely designed to bind to the subject binding pockets.

The test compound may be screened as part of a library or a data base of molecules. Modulators of a binding pocket of the present invention may be identified by docking a computer representation of compounds from one or more database of molecules. Data bases which may be used include ACD (Molecular Designs Limited), NCI (National Cancer Institute), CCDC (Cambridge Crystallographic Data Center), CAST (Chemical Abstract Service), Derwent (Derwent Information Limited), Maybridge (Maybridge Chemical Company Ltd), Aldrich (Aldrich Chemical Company), DOCK (University of California in San Francisco), and the Directory of Natural Products (Chapman & Hall). Computer programs such as CONCORD (Tripos Associates) or DB-Converter (Molecular Simulations Limited) can be used to convert a data set represented in two dimensions to one represented in three dimensions.

Test compounds may tested for their capacity to fit spatially into a binding pocket. As used herein, the term "fits spatially" means that the three-dimensional structure of the test compound is accommodated geometrically in a cavity of a binding pocket. The test compound can then be considered to be a ligand.

A favourable geometric fit occurs when the surface area of the test compound is in close proximity with the surface area of the cavity of a binding pocket without forming unfavorable interactions. A favourable complementary interaction occurs where the test compound interacts by hydrophobic, aromatic, ionic, dipolar, or hydrogen donating and accepting forces. Unfavourable interactions may be steric hindrance between atoms in the test compound and atoms in the binding pocket.

If a model of the present invention is a computer model, the test compounds may be positioned in a binding pocket through computational docking. If, on the other hand, the model of the present invention is a structural model, the test compounds may be positioned in the binding pocket by, for example, manual docking.

As used herein the term "docking" refers to a process of placing a compound in close proximity with a binding pocket, or a process of finding low energy conformations of a test compound/ binding pocket complex.

A screening method of the present invention may comprise the following steps:

(i) generating a computer model of a binding pocket using a crystal according to the invention;

(ii) docking a computer representation of a test compound with the computer model; and

(iii) analysing the fit of the compound in the binding pocket.

In an aspect of the invention, a method is provided comprising the following steps:

(a) docking a computer representation of a structure of a test compound into a computer representation of a binding pocket defined in accordance with the invention using a computer program, or by interactively moving the representation of the test compound into the representation of the binding pocket;

(b) characterizing the geometry and the complementary interactions formed between the atoms of the binding pocket and the compound; optionally

(c) searching libraries for molecular fragments which can fit into the empty space between the compound and the binding pocket and can be linked to the compound; and

(d) linking the fragments found in (c) to the compound and evaluating the new modified compound.

In an embodiment of the invention, a method is provided which comprises the following steps:

(a) docking a computer representation of a test compound from a computer data base with a computer representation of a selected binding pocket defined in accordance with the invention to define a complex;

(b) determining a conformation of the complex with a favorable fit and favourable complementary interactions; and

(c) identifying test compounds that best fit the selected binding pocket as potential modulators of a F-box protein or SCF complex comprising the binding pocket.

In another embodiment of the invention, a method is provided which comprises docking a computer representation of a selected binding pocket defined by the atomic interactions, atomic contacts, or structural coordinates in accordance with the invention to define a complex. In particular a method is provided comprising:

(a) docking a computer representation of a test compound from a computer database with a computer representation of a selected binding pocket defined by the atomic interactions, atomic contacts, or structural coordinates described herein;

(b) determining a conformation of the complex with a favorable fit and favourable complementary interactions; and

(c) identifying test compounds that best fit the selected binding pocket as potential modulators of the a F-box protein or SCF complex comprising the binding pocket

A model used in a screening method may comprise a binding pocket either alone or in association with one or more ligands and/or cofactors. For example, the model may comprise the binding pocket in association with a substrate (or analogue thereof), and/or modulator.

If the model comprises an unassociated binding pocket, then the selected site under investigation may be the binding pocket itself. The test compound may, for example, mimic a known ligand (e.g. substrate) for an F-box protein in order to interact with the binding pocket. The selected site may alternatively be another site on the F-box protein.

If the model comprises an associated binding pocket, for example a binding pocket in association with a substrate or ligand, the selected site may be the binding pocket or a site made up of the binding pocket and the complexed substrate or ligand, or a site on the substrate or ligand itself. The test compound may be investigated for its capacity to modulate the interaction with the associated molecule.

The screening methods described herein may be applied to a plurality of test compounds, to identify those that best fit the selected site. A test compound (or plurality of test compounds) may be selected on the basis of their similarity to a substrate or ligand for an F-box protein. For example, the screening method may comprise the following steps:

(i) generating a computer model of a binding pocket in complex with a substrate or ligand;

(ii) searching for a test compound with a similar three dimensional structure and/or similar chemical groups as the substrate or ligand; and

(iii) evaluating the fit of the test compound in the binding pocket.

Searching may be carried out using a database of computer representations of potential compounds, using methods known in the art.

The present invention also provides a method for designing ligands for F-box proteins or SCF complexes. It is well known in the art to use a screening method as described above to identify a test compound with promising fit, but then to use this test compound as a starting point to design a ligand with improved fit to the model. Such techniques are known as "structure–based ligand design" (See Kuntz et al., 1994, Acc. Chem. Res. 27:117; Guida, 1994, Current Opinion in Struc. Biol. 4: 777; and Colman, 1994, Current Opinion in Struc. Biol. 4: 868, for reviews of structure-based drug design and identification;and Kuntz et al 1982, J. Mol. Biol. 162:269; Kuntz et al., 1994, Acc. Chem. Res. 27: 117; Meng et al., 1992, J. Compt. Chem. 13: 505; Bohm, 1994, J. Comp. Aided Molec. Design 8: 623 for methods of structure-based modulator design).

Examples of computer programs that may be used for structure-based ligand design are CAVEAT (Bartlett et al., 1989, in "Chemical and Biological Problems in Molecular Recognition", Roberts, S.M. Ley, S.V.; Campbell, N.M. eds; Royal Society of Chemistry: Cambridge, pp 182-196); FLOG (Miller et al., 1994, J. Comp. Aided Molec. Design 8:153); PRO Modulator (Clark et al., 1995 J. Comp. Aided Molec. Design 9:13); MCSS (Miranker and Karplus, 1991, Proteins: Structure, Fuction, and Genetics 8:195); and, GRID (Goodford, 1985, J. Med. Chem. 28:849).

The method may comprise the following steps:

(i) docking a model of a test compound with a model of a binding pocket;

(ii) identifying one or more groups on the test compound which may be modified to improve their fit in the binding pocket;

(iii) replacing one or more identified groups to produce a modified test compound model; and

(iv) docking the modified test compound model with the model of the binding pocket.

Evaluation of fit may comprise the following steps:

(a) mapping chemical features of a test compound such as by hydrogen bond donors or acceptors, hydrophobic/lipophilic sites, positively ionizable sites, or negatively ionizable sites; and

(b) adding geometric constraints to selected mapped features.

The fit of the modified test compound may then be evaluated using the same criteria.

The chemical modification of a group may either enhance or reduce hydrogen bonding interaction, charge interaction, hydrophobic interaction, Van Der Waals interaction or dipole interaction between the test compound and the key amino acid residue(s) of the binding pocket. Preferably the group modifications involve the addition removal or replacement of substituents onto the test compound such that the substituents are positioned to collide or to bind

preferentially with one or more amino acid residues that correspond to the key amino acid residues of the binding pocket.

If a modified test compound model has an improved fit, then it may bind to a binding pocket and be considered to be a "ligand". Rational modification of groups may be made with the aid of libraries of molecular fragments which may be screened for their capacity to fit into the available space and to interact with the appropriate atoms. Databases of computer representations of libraries of chemical groups are available commercially, for this purpose.

The test compound may also be modified "*in situ*" (i.e. once docked into the potential binding pocket), enabling immediate evaluation of the effect of replacing selected groups. The computer representation of the test compound may be modified by deleting a chemical group or groups, or by adding a chemical group or groups. After each modification to a compound, the atoms of the modified compound and potential binding pocket can be shifted in conformation and the distance between the modulator and the binding pocket atoms may be scored on the basis of geometric fit and favourable complementary interactions between the molecules. This technique is described in detail in Molecular Simulations User Manual, 1995 in LUDI.

Examples of ligand building and/or searching computer programs include programs in the Molecular Simulations Package (Catalyst), ISIS/HOST, ISIS/BASE, and ISIS/DRAW (Molecular Designs Limited), and UNITY (Tripos Associates).

The "starting point" for rational ligand design may be a known substrate or lignad.. For example, in order to identify potential modulators of an F-box protein, a logical approach would be to start with a known ligand or substrate to produce a molecule which mimics the binding of the ligand or substrate. Such a molecule may, for example, act as a competitive inhibitor for the true substrate or ligand, or may bind so strongly that the interaction (and inhibition) is effectively irreversible.

Such a method may comprise the following steps:

(i) generating a computer model of a binding pocket in complex with a substrate or ligand;

(ii) replacing one or more groups on the ligand model to produce a modified substrate or ligand; and

(iii) evaluating the fit of the modified substrate or ligand in the binding pocket.

The replacement groups could be selected and replaced using a compound construction program which replaces computer representations of chemical groups with groups from a computer database, where the representations of the compounds are defined by structural coordinates.

In an embodiment, a screening method is provided for identifying a substrate or ligand of an F-box protein, comprising the step of using the structural coordinates of a CPD motif defined in relation to its spatial association with a binding pocket of the invention, to generate a compound that is capable of associating with the binding pocket.

In an embodiment of the invention, a screening method is provided for identifying a ligand of an F-box protein, in particular a cdc4 protein, comprising the step of using the structural coordinates of the CPD motif listed in Table 6 to generate a compound for associating with a binding pocket of an F-box protein, in particular a cdc4 protein

as described herein. The following steps are employed in a particular method of the invention: (a) generating a computer representation of a CPD motif defined by its structural coordinates listed in Table 6; and (b) searching for molecules in a data base that are structurally or chemically similar to the defined CPD motif, using a searching computer program, or replacing portions of the CPD motif with similar chemical structures from a database using a compound building computer program.

A screening method is provided for identifying a ligand of an F-box protein, in particular a cdc4 protein, or a SCF complex comprising the step of using the structural coordinates of a binding pocket comprising a WD40 repeat or part thereof listed in Table 6 to generate a compound for associating with a F-box domain of an F-box protein. The following steps are employed in a particular method of the invention: (a) generating a computer representation of a binding pocket comprising a WD40 repeat region or part thereof defined by its structural coordinates listed in Table 6; and (b) searching for molecules in a data base that are structurally or chemically similar to the defined binding pocket using a searching computer program, or replacing portions of the binding pocket with structures from a database using a compound building computer program.

A screening method is provided for identifying a ligand of an F-box protein, in particular a cdc4 protein, of a SCF complex comprising the step of using the structural coordinates of a binding pocket comprising an F-box domain or part thereof, or helical linker listed in Table 6 to generate a compound for associating with a F-box domain or helical linker of an F-box protein. The following steps are employed in a particular method of the invention: (a) generating a computer representation of a binding pocket comprising a an F-box domain or part thereof, or helical linker defined by its structural coordinates listed in Table 4; and (b) searching for molecules in a data base that are structurally or chemically similar to the defined binding pocket using a searching computer program, or replacing portions of the binding pocket with structures from a database using a compound building computer program.

The screening methods of the present invention may be used to identify compounds or entities that associate with a molecule that associates with an F-box protein, in particular a cdc4 protein, or an SCF complex.

In an illustrative embodiment, the design of potential modulators or substrates for SCF complexes begins from the general perspective of shape complimentarity for an active site and substrate specificity subsites of the receptor, and a search algorithm is employed which is capable of scanning a database of small molecules of known three-dimensional structure for candidates which fit geometrically into the target protein site. It is not expected that the molecules found in the shape search will necessarily be leads themselves, since no evaluation of chemical interaction need necessarily be made during the initial search. Rather, it is anticipated that such candidates might act as the framework for further design, providing molecular skeletons to which appropriate atomic replacements can be made. Of course, the chemical complimentarity of these molecules can be evaluated, but it is expected that atom types will be changed to maximize the electrostatic, hydrogen bonding, and hydrophobic interactions with the receptor. Most algorithms of this type provide a method for finding a wide assortment of chemical structures that are complementary to the shape of a binding site of a subject molecule or complex. Each of a set of small molecules from a particular data-base, such as the Cambridge Crystallographic Data Bank (CCDB) (Allen et al. (1973) *J. Chem. Doc.*

13: 119), is individually docked to the binding pocket of the invention, in a number of geometrically permissible orientations with use of a docking algorithm. In a preferred embodiment, a set of computer algorithms called DOCK, can be used to characterize the shape of invaginations and grooves that form active sites and recognition surfaces of a subject molecule or complex(Kuntz et al. (1982) *J. Mol. Biol* 161: 269-288). The program can also search a database of small molecules for templates whose shapes are complementary to particular binding pockets or sites of a receptor (DesJarlais et al. (1988) *J Med Chem* 31: 722-729). These templates normally require modification to achieve good chemical and electrostatic interactions (DesJarlais et al. (1989) *ACS Symp Ser* 413: 60-69). However, the program has been shown to position accurately known cofactors for ligands based on shape constraints alone.

The orientations are evaluated for goodness-of-fit and the best are kept for further examination using molecular mechanics programs, such as AMBER or CHARMM. Such algorithms have previously proven successful in finding a variety of molecules that are complementary in shape to a given binding site of a molecule or complex, and have been shown to have several attractive features. First, such algorithms can retrieve a remarkable diversity of molecular architectures. Second, the best structures have, in previous applications to other proteins, demonstrated impressive shape complementarity over an extended surface area. Third, the overall approach appears to be quite robust with respect to small uncertainties in positioning of the candidate atoms.

Goodford (1985, *J Med Chem* 28:849-857) and Boobbyer et al. (1989, *J Med Chem* 32:1083-1094) have produced a computer program (GRID) which seeks to determine regions of high affinity for different chemical groups (termed probes) on the molecular surface of the binding site. GRID hence provides a tool for suggesting modifications to known ligands that might enhance binding. It may be anticipated that some of the sites discerned by GRID as regions of high affinity correspond to "pharmacophoric patterns" determined inferentially from a series of known ligands. As used herein, a pharmacophoric pattern is a geometric arrangement of features of the anticipated ligand that is believed to be important for binding. Attempts have been made to use pharmacophoric patterns as a search screen for novel ligands (Jakes et al. (1987) *J Mol Graph* 5:41-48; Brint et al. (1987) *J Mol Graph* 5:49-56; Jakes et al. (1986) *J Mol Graph* 4:12-20); however, the constraint of steric and "chemical" fit in the putative (and possibly unknown) binding pocket or site is ignored. Goodsell and Olson (1990, *Proteins: Struct Funct Genet* 8:195-202) have used the Metropolis (simulated annealing) algorithm to dock a single known ligand into a target protein. They allow torsional flexibility in the ligand and use GRID interaction energy maps as rapid lookup tables for computing approximate interaction energies. Given the large number of degrees of freedom available to the ligand, the Metropolis algorithm is time-consuming and is unsuited to searching a candidate database of a few thousand small molecules.

Yet a further embodiment of the present invention utilizes a computer algorithm such as CLIX which searches such databases as CCDB for small molecules which can be oriented in a binding pocket or site in a way that is both sterically acceptable and has a high likelihood of achieving favorable chemical interactions between the candidate molecule and the surrounding amino acid residues. The method is based on characterizing a binding pocket in terms of an ensemble of favorable binding positions for different chemical groups and then searching for

orientations of the candidate molecules that cause maximum spatial coincidence of individual candidate chemical groups with members of the ensemble. The current availability of computer power dictates that a computer-based search for novel ligands follows a breadth-first strategy. A breadth-first strategy aims to reduce progressively the size of the potential candidate search space by the application of increasingly stringent criteria, as opposed to a depth-first strategy wherein a maximally detailed analysis of one candidate is performed before proceeding to the next. CLIX conforms to this strategy in that its analysis of binding is rudimentary -it seeks to satisfy the necessary conditions of steric fit and of having individual groups in "correct" places for bonding, without imposing the sufficient condition that favorable bonding interactions actually occur. A ranked "shortlist" of molecules, in their favored orientations, is produced which can then be examined on a molecule-by-molecule basis, using computer graphics and more sophisticated molecular modeling techniques. CLIX is also capable of suggesting changes to the substituent chemical groups of the candidate molecules that might enhance binding.

The algorithmic details of CLIX is described in Lawerence et al. (1992) *Proteins* 12:31-41, and the CLIX algorithm can be summarized as follows. The GRID program is used to determine discrete favorable interaction positions (termed target sites) in the binding pocket or site of the protein for a wide variety of representative chemical groups. For each candidate ligand in the CCDB an exhaustive attempt is made to make coincident, in a spatial sense in the binding site of the protein, a pair of the candidate's substituent chemical groups with a pair of corresponding favorable interaction sites proposed by GRID. All possible combinations of pairs of ligand groups with pairs of GRID sites are considered during this procedure. Upon locating such coincidence, the program rotates the candidate ligand about the two pairs of groups and checks for steric hindrance and coincidence of other candidate atomic groups with appropriate target sites. Particular candidate/orientation combinations that are good geometric fits in the binding site and show sufficient coincidence of atomic groups with GRID sites are retained.

Consistent with the breadth-first strategy, this approach involves simplifying assumptions. Rigid protein and small molecule geometry is maintained throughout. As a first approximation rigid geometry is acceptable as the energy minimized coordinates of a deduced structure, describe an energy minimum for the molecule, albeit a local one. If the surface residues of the site of interest are not involved in crystal contacts then the crystal configuration of those residues is used merely as a starting point for energy minimization, and potential solution structures for those residues determined. The deduced structure should reasonably mimic the mean solution configuration.

A further assumption implicit in CLIX is that the potential ligand, when introduced into the binding pocket or site of a receptor, does not induce change in the protein's stereochemistry or partial charge distribution and so alter the basis on which the GRID interaction energy maps were computed. It must also be stressed that the interaction sites predicted by GRID are used in a positional and type sense only, i.e., when a candidate atomic group is placed at a site predicted as favorable by GRID, no check is made to ensure that the bond geometry, the state of protonation, or the partial charge distribution favors a strong interaction between the protein and that group. Such detailed analysis should form part of more advanced modeling of candidates identified in the CLIX shortlist.

Yet another embodiment of a computer-assisted molecular design method for identifying ligands of a binding pocket of the invention comprises the *de novo* synthesis of potential ligands by algorithmic connection of small molecular fragments that will exhibit the desired structural and electrostatic complementarity with an active site or binding pocket of the receptor. The methodology employs a large template set of small molecules with are iteratively pieced together in a model of a binding pocket. Each stage of ligand growth is evaluated according to a molecular mechanics-based energy function, which considers van der Waals and coulombic interactions, internal strain energy of the lengthening ligand, and desolvation of both ligand and receptor. The search space can be managed by use of a data tree that is kept under control by pruning according to the binding criteria.

In an illustrative embodiment, the search space is limited to consider only amino acids and amino acid analogs as the molecular building blocks. Such a methodology generally employs a large template set of amino acid conformations, though need not be restricted to just the 20 natural amino acids, as it can easily be extended to include other related fragments of interest to the medicinal chemist, e.g. amino acid analogs. The putative ligands that result from this construction method are peptides and peptide-like compounds rather than the small organic molecules that are typically the goal of drug design research. The appeal of the peptide building approach is not that peptides are preferable to organics as potential pharmaceutical agents, but rather that: (1) they can be generated relatively rapidly de novo; (2) their energetics can be studied by well-parameterized force field methods; (3) they are much easier to synthesize than are most organics; and (4) they can be used in a variety of ways, for peptidomimetic ligand design, protein-protein binding studies, and even as shape templates in the more commonly used 3D organic database search approach described above.

Such a *de novo* peptide design method has been incorporated in a software package called GROW (Moon et al. (1991) *Proteins* 11:314-328). In a typical design session, standard interactive graphical modeling methods are employed to define the structural environment in which GROW is to operate. For instance, environment could be an active site binding pocket of an F-box protein, or it could be a set of features on the protein's surface to which the user wishes to bind a peptide-like molecule. The GROW program then operates to generate a set of potential ligand molecules. Interactive modeling methods then come into play again, for examination of the resulting molecules, and for selection of one or more of them for further refinement.

To illustrate, GROW operates on an atomic coordinate file generated by the user in the interactive modeling session, such as the coordinates provided in Table 4, or the coordinates of a binding pocket or active site as described in Tables 2 and 4 plus a small fragment (e.g., an acetyl group) positioned in the active site to provide a starting point for peptide growth. These are referred to as "site" atoms and "seed" atoms, respectively. A second file provided by the user contains a number of control parameters to guide the peptide growth (Moon et al. (1991) *Proteins* 11:314-328).

The operation of the GROW algorithm is conceptually fairly simple. GROW proceeds in an iterative fashion, to systematically attach to the seed fragment each amino acid template in a large preconstructed library of amino acid conformations. When a template has been attached, it is scored for goodness-of-fit to the receptor site or

binding pocket, and then the next template in the library is attached to the seed. After all the templates have been tested, only the highest scoring ones are retained for the next level of growth. This procedure is repeated for the second growth level; each library template is attached in turn to each of the bonded seed/amino acid molecules that were retained from the first step, and then scored. Again, only the best of the bonded seed/dipeptide molecules that result are retained for the third level of growth. The growth of peptides can proceed in the N-to-C direction only, the reverse direction only, or in alternating directions, depending on the initial control specifications supplied by the user. Successive growth levels therefore generate peptides that are lengthened by one residue. The procedure terminates when the user-defined peptide length has been reached, at which point the user can select from the constructed peptides those to be studied further. The resulting data provided by the GROW procedure includes not only residue sequences and scores, but also atomic coordinates of the peptides, related directly to the coordinate system of the binding site atoms.

In yet another embodiment, potential pharmacophoric compounds can be determined using a method based on an energy minimization-quenched molecular dynamics algorithm for determining energetically favorable positions of functional groups in the binding pockets of the invention. The method can aid in the design of molecules that incorporate such functional groups by modification of known ligands or *de novo* construction.

For example, the multiple copy simultaneous search method (MCSS) described by Miranker et al. (1991) *Proteins* 11: 29-34 may be employed. To determine and characterize a local minima of a functional group in the forcefield of the protein, multiple copies of selected functional groups are first distributed in a binding pocket of interest on the F-box protein. Energy minimization of these copies by molecular mechanics or quenched dynamics yields the distinct local minima. The neighborhood of these minima can then be explored by a grid search or by constrained minimization. In one embodiment, the MCSS method uses the classical time dependent Hartee (TDH) approximation to simultaneously minimize or quench many identical groups in the forcefield of the protein.

Implementation of the MCSS algorithm requires a choice of functional groups and a molecular mechanics model for each of them. Groups must be simple enough to be easily characterized and manipulated (3-6 atoms, few or no dihedral degrees of freedom), yet complex enough to approximate the steric and electrostatic interactions that the functional group would have in binding to the pocket or site of interest in the F-box protein. A preferred set is, for example, one in which most organic molecules can be described as a collection of such groups (*Patai's Guide to the Chemistry of Functional Groups*, ed. S. Patai (New York: John Wiley, and Sons, (1989)). This includes fragments such as acetonitrile, methanol, acetate, methyl ammonium, dimethyl ether, methane, and acetaldehyde.

Determination of the local energy minima in the binding pocket or site requires that many starting positions be sampled. This can be achieved by distributing, for example, 1,000-5,000 groups at random inside a sphere centered on the binding site; only the space not occupied by the protein needs to be considered. If the interaction energy of a particular group at a certain location with the protein is more positive than a given cut-off (e.g. 5.0 kcal/mole) the group is discarded from that site. Given the set of starting positions, all the fragments are minimized simultaneously by use of the TDH approximation (Elber et al. (1990) *J Am Chem Soc* 112: 9161-9175). In this method, the forces on

each fragment consist of its internal forces and those due to the protein. The essential element of this method is that the interactions between the fragments are omitted and the forces on the protein are normalized to those due to a single fragment. In this way simultaneous minimization or dynamics of any number of functional groups in the field of a single protein can be performed.

Minimization is performed successively on subsets of, for example 100, of the randomly placed groups. After a certain number of step intervals, such as 1,000 intervals, the results can be examined to eliminate groups converging to the same minimum. This process is repeated until minimization is complete (e.g. RMS gradient of 0.01 kcal/mole/C). Thus the resulting energy minimized set of molecules comprises what amounts to a set of disconnected fragments in three dimensions representing potential pharmacophores.

The next step then is to connect the pharmacophoric pieces with spacers assembled from small chemical entities (atoms, chains, or ring moieties). In a preferred embodiment, each of the disconnected can be linked in space to generate a single molecule using such computer programs as, for example, NEWLEAD (Tschinke et al. (1993) *J Med Chem* 36: 3863,3870). The procedure adopted by NEWLEAD executes the following sequence of commands: (1) connect two isolated moieties, (2) retain the intermediate solutions for further processing, (3) repeat the above steps for each of the intermediate solutions until no disconnected units are found, and (4) output the final solutions, each of which is a single molecule. Such a program can use for example, three types of spacers: library spacers, single-atom spacers, and fuse-ring spacers. The library spacers are optimized structures of small molecules such as ethylene, benzene and methylamide. The output produced by programs such as NEWLEAD consist of a set of molecules containing the original fragments now connected by spacers. The atoms belonging to the input fragments maintain their original orientations in space. The molecules are chemically plausible because of the simple makeup of the spacers and functional groups, and energetically acceptable because of the rejection of solutions with van-der Waals radii violations.

Compounds and entities (e.g. ligands) of F-box proteins, in particular cdc4 proteins, or SCF complexes identified using the above-described methods may be prepared using methods described in standard reference sources utilized by those skilled in the art. For example, organic compounds may be prepared by organic synthetic methods described in references such as March, 1994, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, New York, McGraw Hill.

Test compounds and ligands which are identified using a crystal or model of the present invention can be screened in assays such as those well known in the art. Screening may be for example *in vitro*, in cell culture, and/or *in vivo*. Biological screening assays preferably centre on activity-based response models, binding assays (which measure how well a compound binds to a binding pocket of a receptor), and bacterial, yeast, and animal cell lines (which measure the biological effect of a compound in a cell). The assays may be automated for high throughput screening in which large numbers of compounds can be tested to identify compounds with the desired activity. The biological assay may also be an assay for the binding activity of a compound that selectively binds to the binding pocket compared to other receptors.

LIGANDS/COMPOUNDS IDENTIFIED BY SCREENING METHODS

The present invention provides a ligand or compound identified by a screening method of the present invention. A ligand or compound may have been designed rationally by using a model according to the present invention. A ligand or compound identified using the screening methods of the invention may specifically associate with a target compound, or part thereof (e.g. a binding pocket). In the present invention the target compound may be the F-box protein or SCF complex or part thereof, or a molecule that is capable of associating with an F-box protein or SCF complex or part thereof (for example a substrate).

A ligand or compound identified using a screening method of the invention may act as a "modulator", i.e. a compound which affects the activity of an F-box protein or SCF complex. A modulator may reduce, enhance or alter the biological function of an F-box protein or an SCF E3 ubiquitin ligase. For example a modulator may modulate the capacity of the F-box protein or an SCF E3 ubiquitin ligase to interact with its substrate. An alteration in biological function may be characterised by a change in specificity. For example, a modulator may cause the F-box protein to interact with a different substrate. In order to exert its function, the modulator commonly binds to a binding pocket.

A "modulator" which is capable of reducing the biological function of the enzyme may also be known as an inhibitor. Preferably an inhibitor reduces or blocks the capacity of the F-box protein or an SCF E3 ubiquitin ligase to interact with its substrate thus reducing or blocking ubiquitination of the substrate. The inhibitor may mimic the binding of a substrate, for example, it may be a substrate analogue. A substrate analogue may be designed by considering the interactions between the substrate and the F-box protein or an SCF E3 ubiquitin ligase (for example, by using information derivable from the crystal of the invention) and specifically altering one or more groups (as described above).

The present invention also provides a method for modulating the activity of an F-box protein, in particular a cdc4 protein, using a modulator according to the present invention. The invention also provides a method for modulating (e.g. potentiating or inhibiting) ubiquitination of a substrate by an SCF E3 ubiquitin ligase, by potentiating or inhibiting the substrate binding pocket of the ligase. Inhibition of ubiquitination of a substrate may decrease signaling and inhibit cellular processes that may be involved in disease. It would be possible to monitor cellular processes following such treatments by a number of methods known in the art.

A modulator may be an agonist, partial agonist, partial inverse agonist or antagonist of an F-box protein.

As mentioned above, a substrate or an identified ligand may act as a ligand model (for example, a template) for the development of other compounds. A modulator may be a mimetic of a substrate or ligand.

Like the test compound (see above) a modulator may be one or a variety of different sorts of molecule. (See examples herein.) A modulator may be an endogenous physiological compound, or it may be a natural or synthetic compound. The term "modulator" also refers to a chemically modified ligand or substrate.

The technique suitable for preparing a modulator will depend on its chemical nature. For example, peptides can be synthesized by solid phase techniques (Roberge JY *et al* (1995) Science 269: 202-204) and automated synthesis may be achieved, for example, using the ABI 43 1 A Peptide Synthesizer (Perkin Elmer) in accordance with

the instructions provided by the manufacturer. Once cleaved from the resin, the peptide may be purified by preparative high performance liquid chromatography (e.g., Creighton (1983) Proteins Structures and Molecular Principles, WH Freeman and Co, New York NY). The composition of the synthetic peptides may be confirmed by amino acid analysis or sequencing (e.g., the Edman degradation procedure; Creighton, *supra*).

If a modulator is a nucleotide, or a polypeptide expressable therefrom, it may be synthesized, in whole or in part, using chemical methods well known in the art (see Caruthers MH *et al* (1980) Nuc Acids Res Symp Ser 215-23, Horn T *et al* (1980) Nuc Acids Res Symp Ser 225-232), or it may be prepared using recombinant techniques well known in the art.

Organic compounds may be prepared by organic synthetic methods described in references such as March, 1994, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, New York, McGraw Hill.

The invention also relates to classes of modulators of F-box proteins, in particular cdc4 proteins based on the structure and shape of a substrate or component thereof, defined in relation to the substrate's spatial association with a crystal structure of the invention or part thereof.

A class of modulators may comprise a compound containing a structure of a CPD motif. In particular, the modulators can comprise a CPD motif having the structural coordinates of the CPD motif in the active site binding pocket of an F-box protein. In an embodiment, a modulator comprises the structural coordinates of a CPD motif having the structural coordinates listed in Table 6.

The invention contemplates all optical isomers and racemic forms of the modulators of the invention.

PHARMACEUTICAL COMPOSITION

The present invention also provides for the use of a modulator according to the invention, in the manufacture of a medicament to treat and/or prevent a disease in a mammalian patient. There is also provided a pharmaceutical composition comprising such a modulator and a method of treating and/or preventing a disease comprising the step of administering such a modulator or pharmaceutical composition to a subject, preferably a mammalian patient.

The pharmaceutical compositions may be for human or animal usage in human and veterinary medicine and will typically comprise a pharmaceutically acceptable carrier, diluent, excipient, adjuvant or combination thereof.

Acceptable carriers or diluents for therapeutic use are well known in the pharmaceutical art, and are described, for example, in Remington's Pharmaceutical Sciences, Mack Publishing Co. (A. R. Gennaro edit. 1985). The choice of pharmaceutical carrier, excipient or diluent can be selected with regard to the intended route of administration and standard pharmaceutical practice. The pharmaceutical compositions may comprise as - or in addition to - the carrier, excipient or diluent any suitable binder(s), lubricant(s), suspending agent(s), coating agent(s), solubilising agent(s).

Preservatives, stabilizers, dyes and even flavouring agents may be provided in the pharmaceutical composition. Examples of preservatives include sodium benzoate, sorbic acid and esters of p-hydroxybenzoic acid. Antioxidants and suspending agents may also be used.

The routes for administration (delivery) include, but are not limited to, one or more of: oral (e.g. as a tablet, capsule, or as an ingestable solution), topical, mucosal (e.g. as a nasal spray or aerosol for inhalation), nasal, parenteral (e.g. by an injectable form), gastrointestinal, intraspinal, intraperitoneal, intramuscular, intravenous, intrauterine, intraocular, intradermal, intracranial, intratracheal, intravaginal, intracerebroventricular, intracerebral, subcutaneous, ophthalmic (including intravitreal or intracameral), transdermal, rectal, buccal, vaginal, epidural, sublingual.

Where the pharmaceutical composition is to be delivered mucosally through the gastrointestinal mucosa, it should be able to remain stable during transit though the gastrointestinal tract; for example, it should be resistant to proteolytic degradation, stable at acid pH and resistant to the detergent effects of bile.

Where appropriate, the pharmaceutical compositions can be administered by inhalation, in the form of a suppository or pessary, topically in the form of a lotion, gel, hydrogel, solution, cream, ointment or dusting powder, by use of a skin patch, orally in the form of tablets containing excipients such as starch or lactose or chalk, or in capsules or ovules either alone or in admixture with excipients, or in the form of elixirs, solutions or suspensions containing flavouring or colouring agents, or they can be injected parenterally, for example intravenously, intramuscularly or subcutaneously. For parenteral administration, the compositions may be best used in the form of a sterile aqueous solution which may contain other substances, for example enough salts or monosaccharides to make the solution isotonic with blood. The aqueous solutions should be suitably buffered (preferably to a pH of from 3 to 9), if necessary. The preparation of suitable parenteral formulations under sterile conditions is readily accomplished by standard pharmaceutical techniques well-known to those skilled in the art.

If the agent of the present invention is administered parenterally, then examples of such administration include one or more of: intravenously, intra-arterially, intraperitoneally, intrathecally, intraventricularly, intraurethrally, intrasternally, intracranially, intramuscularly or subcutaneously administering the agent; and/or by using infusion techniques.

For buccal or sublingual administration the compositions may be administered in the form of tablets or lozenges which can be formulated in a conventional manner.

The tablets may contain excipients such as microcrystalline cellulose, lactose, sodium citrate, calcium carbonate, dibasic calcium phosphate and glycine, disintegrants such as starch (preferably corn, potato or tapioca starch), sodium starch glycollate, croscarmellose sodium and certain complex silicates, and granulation binders such as polyvinylpyrrolidone, hydroxypropylmethylcellulose (HPMC), hydroxypropylcellulose (HPC), sucrose, gelatin and acacia. Additionally, lubricating agents such as magnesium stearate, stearic acid, glyceryl behenate and talc may be included.

Solid compositions of a similar type may also be employed as fillers in gelatin capsules. Preferred excipients in this regard include lactose, starch, cellulose, milk sugar or high molecular weight polyethylene glycols. For aqueous suspensions and/or elixirs, the agent may be combined with various sweetening or flavouring agents,

colouring matter or dyes, with emulsifying and/or suspending agents and with diluents such as water, ethanol, propylene glycol and glycerin, and combinations thereof.

As indicated, a therapeutic agent (e.g. modulator) of the present invention can be administered intranasally or by inhalation and is conveniently delivered in the form of a dry powder inhaler or an aerosol spray presentation from a pressurised container, pump, spray or nebuliser with the use of a suitable propellant, e.g. dichlorodifluoromethane, trichlorofluoromethane, dichlorotetrafluoroethane, a hydrofluoroalkane such as 1,1,1,2-tetrafluoroethane (HFA 134A^{TM}) or 1,1,1,2,3,3,3-heptafluoropropane (HFA 227EA^{TM}), carbon dioxide or other suitable gas. In the case of a pressurised aerosol, the dosage unit may be determined by providing a valve to deliver a metered amount. The pressurised container, pump, spray or nebuliser may contain a solution or suspension of the active compound, e.g. using a mixture of ethanol and the propellant as the solvent, which may additionally contain a lubricant, e.g. sorbitan trioleate. Capsules and cartridges (made, for example, from gelatin) for use in an inhaler or insufflator may be formulated to contain a powder mix of the agent and a suitable powder base such as lactose or starch.

Therapeutic administration of polypeptide modulators may also be accomplished using gene therapy. A nucleic acid including a promoter operatively linked to a heterologous polypeptide may be used to produce high-level expression of the polypeptide in cells transfected with the nucleic acid. DNA or isolated nucleic acids may be introduced into cells of a subject by conventional nucleic acid delivery systems. Suitable delivery systems include liposomes, naked DNA, and receptor-mediated delivery systems, and viral vectors such as retroviruses, herpes viruses, and adenoviruses.

APPLICATIONS

The invention further provides a method of treating a mammal, the method comprising administering to a mammal a modulator or pharmaceutical composition of the present invention.

In particular, the invention contemplates a method of treating or preventing a condition or disease associated with an F-box protein or SCF complex in a cellular organism, comprising:

(a) administering a modulator of the invention in an acceptable pharmaceutical preparation; and

(b) activating or inhibiting an F-box protein or SCF complex or their interaction with a substrate to treat or prevent the disease.

The invention provides for the use of a modulator identified by the methods of the invention in the preparation of a medicament to treat or prevent a disease in a cellular organism. Use of modulators of the invention to manufacture a medicament is also provided.

Typically, a physician will determine the actual dosage of a modulator or pharmaceutical composition of the invention that will be most suitable for an individual subject and it will vary with the age, weight and response of the particular patient and severity of the condition. There can, of course, be individual instances where higher or lower dosage ranges are merited.

The specific dose level and frequency of dosage for any particular patient may be varied and will depend upon a variety of factors including the activity of the specific compound employed, the metabolic stability and length of action of that compound, the age, body weight, general health, sex, diet, mode and time of administration, rate of

excretion, drug combination, the severity of the particular condition, and the individual undergoing therapy. By way of example, the pharmaceutical composition of the present invention may be administered in accordance with a regimen of 1 to 10 times per day, such as once or twice per day.

For oral and parenteral administration to human patients, the daily dosage level of the agent may be in single or divided doses.

The modulators and compositions of the invention may be useful in the prevention and treatment of conditions involving aberrant F-box proteins or SCF complexes. In particular the modulators and compositions may be useful in treating cancer or Alzheimer's Disease.

Conditions which may be prevented or treated in accordance with the invention include but are not limited to lymphoproliferative conditions, and malignant and pre-malignant conditionss. Malignant and pre-malignant conditions may include solid tumors, B cell lymphomas, chronic lymphocytic leukemia, chronic myelogenous leukemia, prostate hypertrophy, Hirschsprung disease, glioblastoma, breast and ovarian cancer, adenocarcinoma of the salivary gland, premyelocytic leukemia, prostate cancer, multiple endocrine neoplasia type IIA and IIB, medullary thyroid carcinoma, papillary carcinoma, papillary renal carcinoma, hepatocellular carcinoma, gastrointestinal stromal tumors, sporadic mastocytosis, acute myeloid leukemia, large cell lymphoma or Alk lymphoma, chronic myeloid leukemia, hematological /solid tumors, papillary thyroid carcinoma, stem cell leukemia/lymphoma syndrome, acute myelogenous leukemia, osteosarcoma, multiple myeloma, preneoplastic liver foci, and resistance to chemotherapy.

Modulators and compositions of the invention may be used to restore function to a mutant F-box protein, in particular a mutant cdc4 polypeptide. Modulators and compositions of the invention, in particular inhibitors may also have utility in treating diseases associated with F-box mutations, in particular cdc4 polypeptide mutations, in combination with other cancer mutations, Notch pathway mutations or presenilin mutations.

A modulator of the invention may be used to promote binding of a substrate to a SCF complex. In an embodiment a modulator that associates (preferably with high affinity) with a binding pocket of a SCF complex as described herein, is linked to an agent that binds to a substrate to be ubiquitinated by a SCF complex. A modulator-agent-substrate complex where the modulator is derived from a binding pocket of an F-box protein as described herein may be used in treating diseases associated with a mutant F-box protein.

Therapeutic efficacy and toxicity of compositions and modulators of the invention may be determined by standard pharmaceutical procedures in cell cultures or with experimental animals, such as by calculating the ED_{50} (the dose therapeutically effective in 50% of the population) or LD_{50} (the dose lethal to 50% of the population) statistics. The therapeutic index is the dose ratio of therapeutic to toxic effects and it can be expressed as the ED_{50}/LD_{50} ratio. Pharmaceutical compositions that exhibit large therapeutic indices are preferred.

The invention will now be illustrated by the following non-limiting examples:

EXAMPLE 1

The following methods were used in the investigation described in the example:

Methods

Cloning, Protein expression and Purification

The Cdc4 fragment employed for crystalization, which is deleted for terminal residues 1 to 262 and 745 to 779, extends from the beginning of the F-box domain to the end of the WD40 repeat domain. The N-terminal deletion removes a poorly conserved sequence of 226 amino acids and a conserved element of approximately 40 residues termed the D-domain that immediately precedes the fbox domain and that has been implicated in molecular multimerization. The C terminal deletion removes residues not conserved amongst different Cdc4 homologues. Both Skp1 and Cdc4 were engineered to remove flexible loops, namely residues 36-55 in Skp1 and residues 601 to 604 and 609 to 624 in Cdc4.

A PCR product containing CDC4(263-744) was cloned into the EheI(SfoI) and BamH1 sites of pPROEX HTb. In parallel, a PCR product containing SKP1Δ37-64 was cloned into the NdeI and BamHI sites of pGEX2T-TEV. An SspI GST-SKP1-containing fragment from this construct was cloned into the StuI site of the Cdc4 construct described above such that CDC4 and SKP1 were in opposite orientations. A non-homologous region in CDC4 encoding amino acids 602-624 was then replaced by the DNA sequence GGCGAACTG [SEQ ID NO. 39], which encodes the shorter peptide sequence Gly-Glu-Leu.

The Cdc4/skp1 complex was expressed in *E. coli* B934 (DE3) cells grown in minimal media suplemented with a mixture of selenomethionine (40 ug/ml) and methionine (0.4ug/ml). Cells were induced with 0.2 mM isopropyl-β -D-thiogalactopyranoside (IPTG) at 15° C overnight. Cell pellets were resuspended in 50 mM hepes pH 7.5, 500 mM NaCl , 10% glycerol, and 5 mM Imidazole, lysed with a cell homogenizer (Emulsiflex C-5, Avistin) followed by a 20 sec sonication (vibra cell, Betatec). The lysate was then clarified by centrifugation at 65 000 x g for 40 min. The supernatant was loaded onto a 5 ml metal chelating column (Pharmacia) and eluted in high imidazole. This fraction was loaded onto a glutathione-sepharose column (Pharmacia) and the bound complex was eluted by overnight digestion with TEV protease (Canadian Life). Eluted protein was dialysed to remove DTT and EDTA and reloaded onto a metal chelating column. The flow through containing the complex was concentrated and applied to a Superdex S 75 gel filtration column (Pharmacia). Fractions containing the complex were concentrated in a buffer containing 10 mM hepes pH 7.5, 250 mM NaCl, and 1 m M DTT.

Crystallization, Data Collection, and Structure Determination

Hanging drops containing 1 μl of 21 mg/ml protein plus 1.2 molar equivilents of the CPD peptide sequence were mixed with equal volumes of reservoir buffer containing 0.1 M Tris pH 8.5, and 1.5 M ammonium sulphate. Crystals were flash frozen in reservoir buffer supplemented with 15% glycerol. Crystals of the space group $P3_2$, (a =107.7Å, b = 107.7Å, c = 168.3Å, α = γ = 90°, β =120°), with two molecules of the complex in the asymmetric unit were obtained at 20°C. A Multiple Anomalous Dispersion (MAD) experiment was performed on a frozen crystal at the Advanced Photon Source (Argonne, IL) (APS) beamline BM 14-B and BM 14-D(λ1 = 0.9798 Å, λ2 = 0.9800 Å, λ3 = 0.9000 Å) using a Quantum 4 ADSC CCD detector. Data processing and reduction was carried out with the HKL program suite (Otwinowski and Minor, 1997). The programs SHARP (de La Fortelle and Bricogne, 1997) and

SnB (Miller et al., 1994) were used in combination to locate and refine 19 of the 22 Se sites. Following density modification with Solomon (Abrahams and Leslie, 1996), a partial model was generated using O (Jones et al., 1991) and refined using CNS (Brunger et al., 1998) to a working R value of 24.09% and a free R value of 28.71%. Pertinent statistics for data collection and refinement are shown in Table 1.

The increased order of the second CPDs may be due to a crystal packing interaction involving the c-terminus of the CPD. While the main chain termini of the second CPD are discernable (Figure 3e), the precise backbone and side chain conformations for the P-2 Leu, P-3 Gly, P+4 Ser, and P+5 Gly are less reliably determined.

Mutagenesis

Point mutants were obtained by a PCR-based approach using oligos provided in supplementary information and Pfu polymerase (Stratagene). Once verified by sequencing the mutants were sub-cloned into the appropriate vectors as listed in the supplementary information. Alanine insertion mutations were obtained using the Kunkel method (ref) and then sub-cloned into the vectors indicated in the supplementary information.

Shuffle experiments

All mutants on a TRP1 ARS CEN plasmid were transformed into a cdc4Δ strain (MT 1259) containing a wildtype copy of CDC4 on a URA3 ARS CEN plasmid. Cells were plated on either Trp^-Ura^- or 5-FOA medium for 2 days at 30° C. Viable cells on 5-FOA were grown in Trp^- medium and transformed with either wild type GAL1-SIC1, GAL1-SIC T45A, or GAL1-SIC T33V on a LEU2 ARS CEN pasmid . Cells were then plated on Leu- Trp- plates containing either glucose or galactose and incubated for 2 days at 30° C.

Sic1-Cdc4 interactions.

Bacterially expressed His6-Sic1 was phosphorylated with Cln2-Cdc28 kinase purified from baculovirus infected Sf9 cells as described before (Nature paper). 1ug of WT or mutant Cdc4-GST-Skp1, immoblized on GSH-Sepharose resin, was incubated with 0.5ug phospho-Sic1 at 4C for 1h and washed 4 times. Captured complexes were resolved on SDS-PAGE and Sic1 visualized by anti-Sic1 Western blotting and ECL. For IEF-2D analysis, several Sic1 phosphorylation reactions were carried out for different time periods to obtain a spectrum of Sic1 that were phosphorylated at different numbers of its nine CDK sites. This pool of phospho-Sic1 (2.5ug) was incubated with 5μg of WT or mutant Cdc4-GST-Skp1 as described above. Different phosphorylation states of Sic1 were separated by denaturing isoelectric focusing (IEF)-2D gel electrophoresis and visualized by anti-Sic1 Western blotting and ECL. IEF was performed using pH3-10NL Immobiline gel strips and IPGphore IEF system (Amersham pharmacia).

Results

The x-ray crystal structure presented herein consists of a ternary complex of yeast Skp1 bound to a fragment of Cdc4, and a 9mer high affinity CPD phosphopeptide (Figure 2). The Cdc4 fragment, which is deleted for terminal residues 1 to 262 and 745 to 779, extends from the beginning of the F-box domain to the end of the WD40 repeat domain.

Skp1- Cdc4 Fbox: Skp1 forms an elongated structure with a mixed α/β topology identical to that reported for human Skp1(Schulman et al, 2000). The topology consists of a three-strand (denoted β1 to β3) β-sheet and eight α-helices,

denoted α1 to α8 (Figure 2a). The structure of Cdc4 from its amino terminus consists of an F-box domain, an α-helical extension or linker, and a WD40 repeat domain (Figure 2a,b). The F-box domain comprises five α helices (denoted α0 to α4). This topology differs slightly from that reported for the F-box domain of hSkp2 (Schulman et al, 2000), which consists of a loop region L1 and three helices denoted α1 to α3. Helix α0 in Cdc4 corresponds most closely in sequence and position to the loop region L1 of Skp2 while a half turn remnant of helix α4 is discernable in the transition sequence between the Skp2 F-box and Leucine Repeat domains. As observed in the Skp1-Skp2 complex, Skp1 and the F-box domain of Cdc4 associate by the interdigiation of helixes α0 to α3of Cdc4 with helices α5 to α8 of Skp1. This mode of inter-domain association is characterized by a common and continuous hydrophobic core that spans the two protein domains.

Cdc4 helical linker and WD40 domain: Following the F-box domain of Cdc4 is a helical extension that forms a structured bridge to the WD40 repeat domain. The helical extension consists of two α-helices α5 and α6 that together with helices α3 and α4 of the F-box domain form a stalk and pedestal like structure that connects and orients the WD40 domain (Figure 2c).

Eight copies of the WD40 repeat motif in Cdc4 form an 8 blade β-propeller structure. Each blade, composed of 4 anti-parallel β-strands, is related by 8-fold pseudo symmetry about a central axis (Figure 2b). As first shown for G-protein gamma subunit (Sondek 1996), the WD40 repeat motif of approximately 40 amino acids composes the outer β-strand of one propeller blade and the inner three strands of the adjacent blade. A continuous circular arrangement of blades is formed by the association of the first and last WD40 repeat motifs to form the 8^{th} propeller blade. Interestingly, a 7 β-propeller blade structure was anticipated for Cdc4 and its orthologues (and generally all WD40 repeat F-box adaptors), which is attributable in part to the cryptic nature of the 8th WD40 repeat motif (Figure 1). Based on the structure based sequence alignment in Figure 1, it is predicted that the other WD40 class of F-box adaptor proteins (i.e. the Met30 orthologues and βTRCP orthologues) will form 7-blade β-propeller structures.

The WD40 repeat domain forms a disk like structure characterized by a cavity in the middle and two opposing circular surfaces of slightly different size. The smaller of the two surfaces composes the CPD binding site. On the bottom surface is anchored helix α6 of the helical extension, which inserts obliquely between propeller blades β7 and β8. Interestingly, β-propeller blade 2 consists of 5 β-strands. The outermost strand of this blade, denoted $\beta 9^1$, is non-standard and arises from an amino acid insert in the connecting loop between β-strands 12 and 13. Strand $\beta 9^1$ forms a parallel arrangement with strand β9, which differs from the anti parallel architecture of all other β-strand elements in the WD40 domain structure. A large insert in the β12-β13 linker is absent from dr, ce, hu, mu Cdc4 homologues suggesting that a 5 βstrand propeller blade 2 is unique to the fungal homologues.

A fixed orientation between the F-box domain and WD40 domain of Cdc4 is maintained largely through the integrity of the stalk like helix α6 of the helical extension (Figure 2c). Helix α6 is 30Å in length, and is anchored at its N-terminus to the hydrophobic core of the F-box/helical extension and at its C-terminus to the hydrophobic core of

the WD40 repeat domain. In contrast to the intermolecular connection between Skp1 and the F-box domain, the connection between the F-box domain and WD40 repeat domain appears less rigidly structured.

At its amino terminus, helix α6 anchors to the F-box through hydrophobic interactions involving α6 residues Phe 355 and Leu 356 and F-box residues Ile 295, and Ile 296, Leu 315, Trp 316, and Leu 319 (Figure 2c). Helix α5 packs along side the base of helix α6 opposite to the F-box domain through hydrophobic packing interactions involving Tyr342, Leu 338 and Leu 334. At its C- terminus, helix α6 anchors through hydrophobic interactions involving residues Trp 365 and Ile 364 with WD repeat residues Val 687, Ile 696, Leu 726 and Phe 743 in β-propeller blades 7 and 8. Asn 364 of helix α6 also forms a tight hydrogen bond interaction with the backbone carbonyl group of Phe 743 in propeller blade 8. The noted interactions (with the exception of interactions involving helix α5) involve residues that are conserved across most WD40 F-box adaptor proteins including the Met30 orthologues and β-TRCP orthologues, which suggests that the linkage between WD40 and F-box domains are similarly structured in these proteins. Helix α6 in β-TRCP, however, appears to be one α-helical turn longer (Figure 1).

Outside of stalk helix α6, only two close contacts (< 3.5Å) are observed between the WD40 repeat domain and other regions of Cdc4. These contacts consist of hydrogen bonds between Asn684 and Arg700 in the loop regions of propeller blade 7 with Glu 323 in the α4-α5 linker of the helical extension. Both, hydrogen bonds are maintained in the two Cdc4 molecules of the crystal asymmetric unit but all three residues are poorly conserved amongst Cdc4 orthologues (Figure 1). The lack of additional stabilizing interactions suggests that the F-box/WD40 domain linkage is not exceedingly rigid, and indeed, the WD40 domain in the two molecules of the asymmetric unit differ relative to their F-box domains by a 5 degree rotation about helix α6.

WD40 domain phosphopeptide recognition: A nine-mer CPD consisting of the sequence acetyl-Gly,Leu,Leu,pThr,Pro,Pro,Gln,Ser,Gly-amide [SEQ ID NO.40] is bound to the front face of the WD40 domain of Cdc4. In the two WD40 repeat domain/CPD complexes of the crystal asymmetric unit, a central core of 4 CPD residues corresponding to the sequence Leu, pThr, Pro, Pro [SEQ ID NO.41] is well ordered.

These residues have been modeled unambiguously in unbiased experimental electron density maps (Figure 3e). Interpretable electron density is also apparent for the P-2 Leu, P-3 Gly, P+3 Gln, P+4 Ser, and P+5Gly positions of the second CPD (no interpretable electron density is apparent for these residues in the first CPD). The CPD binds in an extended manner across β-propeller blade 2 with the N-terminus oriented towards the central cavity of the WD40 repeat domain and the C-terminus oriented towards the outer rim. The CPD binding surface of Cdc4 is composed of invariant and highly conserved residues from β-propeller blades 1 to 6 and 8 and represents the most conserved part of the WD40 repeat domain surface (Figure 3a,c).

Cdc4 displays an absolute requirement for phosphorylation at Ser or Thr at the P-0 position of the CPD. In the crystal structure, the P0 pThr phosphate group is coordinated by an intricate network of electrostatic interactions and hydrogen bonds involving residues absolutely conserved across all Cdc4 orthologues (Figure 3c). The P0 phosphate group forms direct electrostatic interactions with the guanidinium groups of Arg 485, Arg 467, and Arg 534

and a direct hydrogen bond with the side chain of Tyr 548. The side chain of Tyr 548 is coordinated by stacking interactions with the guanidinium group of Arg 572, which in turn is coordinated by a hydrogen bond to the side chain of Tyr 574. Although Cdc4 shows a strong (6 fold) preference for pThr over pSer, the structural basis for this selectivity is not obvious. In the crystal structure, the Cγ methyl group of Thr is directed towards solvent and does not make contact with the CPD binding surface of Cdc4. This binding preference may be due to the greater side chain rotational stability arising from the Thr β-branch structure.

Cdc4 displays an absolute requirement for proline in the p+1 CPD position. In the crystal structure, the P+1 proline side chain projects into a three-sided pocket on the CPD binding surface. The side chain of Trp 426 forms one side of the pocket and packs in a coplanar manner with the P+1 proline side chain. On its other side, the Trp 426 side chain packs tightly against the side chain of Thr 386. The opposite side of the P+1 binding pocket is formed by the side chain of Arg 485. Arg 485 coordinates the P+1 Proline through van der Wals side chain interactions and through a direct hydrogen bond to the Proline backbone carbonyl group. This represents the sole direct hydrogen bond interaction between Cdc4 and the CPD main chain. The side chains of Thr 441 and Thr 465 define the remaining side of the P+1 Proline binding pocket, with the Cγ side chain groups composing a hydrophobic surface. The hydroxyl groups of Thr 441 and 465 orient away from the P+1 binding pocket, where they are well placed to influence binding specificity for CPD residues C-terminal to the P+1 position. Unlike Trp 426, Thr 386 and Arg 485, which are invariant amongst the Cdc4 orthologues, Thr 441 and Thr 465 are substituted with Ile in the S. pombe Cdc4 orthologue Pop1. The modeling studies suggest that this substitution has no effect on the P+1 binding pocket but may perturb CPD binding specificity C-terminal to the P+1 positions through steric effects (Ile is bigger than Thr) and by increasing the hydrophobic character of the surface.

Cdc4 displays a strong preference for the hydrophobic residues Leu, Ile and Proline at the P–1 and P–2 CPD positions. In the crystal structure, the P-1 Leucine side-chain is oriented towards a hydrophobic pocket composed of invariant residues Trp 426, Trp 717, and Thr 386, and the conserved hydrophobic residue Val 384. While less precisely modeled, the main chain position of Leu +2 lies in close proximity to a third hydrophobic pocket composed of the invariant residue Tyr574, and the conserved hydrophobic residues Met 590 and Leu634.

Cdc4 displays little preference for residues in the P+2 to P+5 CPD positions. In the crystal structure, the side chain of P+2 Pro is directed towards solvent (which would account for the lack of selectivity at this position), while the main chain conformation of Pro +1 and Pro+2, causes the CPD to kink away from the peptide-binding surface from the Pro+2 position onwards. As a result, only one additional close contact with Cdc4 is made by the CPD following the Pro +1 position, which consists of a weak hydrogen bond (sub-optimal geometry) between the P+4 Gln side chain and the side chain of Arg 485.

Adjacent to the P+1 proline binding pocket, Ser 464, Thr 441 and Thr 465 are well placed to exert specificity for the +3 and +4 CPD positions if an extended rather than kinked conformation of the CPD were adopted. As noted, Thr 441 and 465 are substituted with Ile in the Cdc4 orthologue pop1 in S. pombe. While nothing is known about the

effect of this substitution on CPD recognition, it is predicted that this could have some effect on substrate selectivity for the P+2 to P+5 CPD positions.

Cdc4 displays strong selectivity against Arginine and Lysine in positions –2, -1, +2, +3 and +4. This selectivity may be due to electrostatic repulsion generated by the invariant Cdc4 residues Arginine 572, 534, 467, 485 and 443, which dominate the local electrostatic character of the CPD binding site. Lys 402 is also well placed to contribute to repulsive effects but this position is not conserved amongst the Cdc4 orthologues. The selectivity against positively charged residues in the P–2 to P–1 CPD positions can also be reconciled in part by the hydrophobic nature of the P-1 and P-2 binding pockets and indeed, oppositely charged Glu and Asp residues are also disfavored at these CPD positions.

Comparison with Skp1-Skp2 complex:

Skp2 is a representative member of a second class of F-box adaptor proteins, which possesses a leucine repeat domain in place of the WD40 repeat of Cdc4. In addition to providing a first structural view of a Skp1 homologue and an F-box domain, the structure of the Skp1/Skp2 complex revealed a mode of molecular association predicted to be employed by all Skp1/F-box homologues. The Cdc4/Skp1/CPD structure confirms the fold of the individual Skp1 and F-box domains and their mode of association. Superposition of yeast and human Skp1 strands β1-β3 and helices α1 to α7 (RMSD Cα = 0.74Å) reveals a close correspondence between F-box helixes α1 to α3 with only Skp1 helix α8 and F-box helix α4 showing significant deviations between the two structures. In addition, only the first half of helix α8 is ordered in ySkp1 and only ha half turn fragment of the F-box helix α4 is apparent in Skp2. The differences in positions and lengths of F-box helices α4 and Skp1 helices α8 reflects the different roles these secondary structure elements play in the linkage between their respective F-box and ligand binding domains.

The structure of the Skp1/Skp2 complex revealed a solid/substantial linkage between its Leucine Repeat and the F-box domains, a feature predicted to be shared by all Skp2 F-box orthologues. In Skp2, the F-box domain helix α4 terminates abruptly and without an appreciable linker, makes an immediate transition to the Leu Repeat domain fold. This linkage is enhanced by a β-strand projecting back from C-terminus of the Leu repeat domain and helix α8 projecting forward from Skp1. The sum of linker region interactions compose a local hydrophobic network that links the hydrophobic cores of the F-box domain with that of the LRR domain. This contrasts sharply with the corresponding linkage of Cdc4, which is composes primarily by a lengthy inter-domain linker (the helical extension) and which lacks significant involvement of Skp1 or the WD40 repeat domain for stabilization.

Although the Skp2 and Cdc4 F-box adaptor proteins employ structurally divergent ligand binding domains, the general position of the WD40 and LLR domains are surprisingly similar. The precise ligand-binding site on Skp2 has not been determined but mutagenesis studies on the Skp2 orthologue in Met30 have mapped the ligand binding site to the inner side of the curved surface. If the Skp2 binding site is inferred from the overlap with the Cdc4 CPD binding site, the CPD site would map to the lateral side of the Leu repeat domain.

Model of the SCF^{Cdc4} E2 complex

The structure of Cdc4 bound to substrate provides a missing piece of the larger SCF structural puzzle and sheds light on how substrate is presented for ubiquitination. A complete model of the SCF^{Cdc4}-E2-substrate complex consisting of an E2, a cullin, a ring finger domain, an F-box adaptor, Skp1, and CPD has been constructed using the structures of individual component proteins and/or larger assemblies determined previously (Figure 4). Two interesting features are apparent. Firstly, a separation distance between the E2 active site cysteine and the peptide-binding site of Cdc4 is very large at 64Å and second Cdc4 presents the CPD peptide with a direct line of sight to the E2.

Mutational analysis of CPD binding surface

In order to probe the functional importance of amino acid residues on the highly conserved peptide binding surface, a panel of Cdc4 mutants (both single and double mutants) were generated and tested each for its ability to bind phospho Sic1 and Skp1 in vitro using a pull down assay and for its ability to substitute for wt-cdc4 in vivo using a cell viability assay. Of 12 single site mutants tested, only Arg 467, Arg485Ala Arg534Ala, and Trp 426 abolished both cell viability in vivo and phosphoSic1 binding in vitro. Together, these residues compose most of the interaction surface with the pThr, Pro CPD core. Interestingly, Tyr 548, the only other amino acid on the surface of CDC4 to directly contact P0 phosphate group, is functional in vivo but is compromised for CPD binding in vitro. Mutation of the adjacent residue Arg572 to Ala shows the same behavior. For the Arg572 mutation, the inablity to bind psic1 in vitro appears due to its tendency to aggregation. Presumably in the context of the full SCF complex in vivo this mutant is sufficiently well behaved to bind phospho Sic1.

All other single site mutants including Arg443Ala, Lys402Ala, Tyr574Ala, Trp717, Val384, and the double site mutant Thr441/465Ile, K404D/R443D and V384N/W717N are viable when expressed in the cdc4 delete and are fully competent for phosphoSic1 binding in vitro.

Since the cell viability assay may be masking subtle functional roles for the conserved Cdc4 residues, function was assayed in vivo under more stringent conditions in which Sic1wt or the stabilized mutants, Sic1(T33V) or Sic1(T45A) are over-expressed under a galactose promoter. This should amplify defects in cdc4 function. Under these conditions, Trp 717, Tyr 548 and the double mutant K404D/R443D are lethal showing that these residues are in fact important for function.

Role of the Stem and pedestal structure

To probe the role of the F-box WD40 inter-domain linker, point mutations, insertions or deletions were introduced into the stem and pedestal structure of Cdc4 and protein function was assessed as performed for the peptide binding site mutants.

Deletion of helix α5 or introduction of Proline and Glycine helix destabilizing residues within the helix had no effect n Cdc4 function both in vitro and in vivo. This result is consistent with the poorly conserved nature f helix α5 and its flanking linker regions. Helix 5 appears entirely absent from human, mouse and drosophila homologues and helix destabilizing substitutions in helix 5, incorporating glycine and proline, are observed in the

worm and fungal homologues (Figure 1). A more invasive deletion of helix 5 that deletes part of the linkers to helix 4 and helix 6 was inviable in yeast. This mutant is properly folded as evidence by the finding that the protein can bind both Skp1 and phospho Sic 1 in vitro. This mutation should likely disrupt the positioning of helix 6 relative to the fbox domain (the linker is too short to span the two secondary structure elements).

The introduction of helix destabilizing residues in helix α6 or the lengthening of the helix by the insertion of one, two, three, four, 8 or 12 amino acid residues also disrupted protein function in vivo, without while maintaining the ability of Cdc4 to to bind pSic1 and Skp1. These results are consistent with a possible role for helix 6 in presenting bound substrates in a specific geometric orientation.

It is peculiar that such a spindly structure is sufficient to maintain rigidity. Perhaps in the context of the dimer, additional contacts help to stabilize position of the WD repeats with respect to the other part of the protein. Indeed, the N terminal dimerization domain is required for function. Or perhaps a modicum of flexibility is important for the catalytic mechanism.

Probing substrate selectivity against positively charged residues

Cdc4 bind Sic1 in a multi site dependent manner. Each of the phosphorylation sites in Sic1 are sub-optimal in isolation but series of 5 to 7, they work coopertively to bind to Cdc4 through an avidity effect. Part of the sub-optimal character of the sites is due to the presence of Lysine in the +2 to +5 positions. From the crystal structure, the selectivity against positive residues appear to arise from electrostatic replusion from highly conserved residues on the CPD binding surface of Cdc4. To test this hypothesis, two residues not directly involved in phosphopeptide binding were mutated and then the multi site requirement for phosphoSic1 binding was evaluated (Figure 5c).

Using an IEF pull down assay, wild type Cdc4 is shown to selectively binds to the 5,6 and 7 site phosphorylated phosphoSic1 from a pool of single to 9 site phosphorylated forms. In contrast, the double mutant binds to 3,4,5,6,7 site phosphorylated forms of Sic1 (Figure 5a). This supports the notion of selectivity and the basis for avidity that may be important for setting sensitive threshold for cell cycle progression (Figure 5b). The same effect was observed for a double mutant.

Cancer causing mutations in drosophila and human Cdc4

Mutations in human and fly orthologues of yCdc4 give rise to cancers (see Table below). All mis-sense mutations map to the WD40 CPD binding domain and either have been demonstrated or are predicted to perturb CPD binding function. In previous studies, two cancer cell lines tested positive for mutations at Arginine 534 and Arg 467 (Arg 534 and Arg 467 in yCdc4). In the crystal structure, these residues make a direct binding interaction with the P0 phospho group and our mutational analysis demonstrates an absolute requirement of these residues for CPD binding. In another study, two entrometrial cancerous tissue samples tested positive for mutations equivalent to Arg467 and Arg 485 in yCdc4. As f r the tumor cell line mutations, these mutations affect key residues required for CPD recogniti n.

Two mutations characterized in drosophila cancer include Ala1118Val and Gly1132Glu, corresponding to yCdc4 positions Ser532 and Gly546 respectively. The first of these mutations, involve the substituti n of a small

Ala/Ser residue with a bulkier b-branched Valine residue. This may compromise CPD binding function through steric effects on the position of Arg434, Arg467, Arg534 triad. In the crystal structure, Ala/Ser is positioned centrally amongst the triad. The second drosophila mutation, Gly1132Glu, maps to β-strand 15 of propeller blade 4 in yCdc4. This position is within the core of the protein and mutation here likely acts by disrupting the overall WD40 domain fold or through local perturbations of structure that indirectly affect the phosphate binding pocket. Glycine in this position of the WD40 repeat motif is highly conserved. The temperature sensitive alleles previously characterized including Gly398Glu in propeller blade 1 and Ser438Asn in propeller blade 2 likely act by disrupting the fold in a similar manner to disrupt the overall WD fold. These are more distantly located from the CPD binding pocket.

Cancer Mutations

H-cell lines	Drosophila	Entrometrial	Orlicky	Rosamond
Arg534(425)Leu Arg 467(385)Cys	Ser/Ala532(1118)Val Gly546(1132)Glu	Arg467(465)His Arg485(479)Gln	Arg534Ala Arg467Ala Arg485Ala Trp426Ala	Gly398Gln Ser438Asn

Discussion

Recognition of phosphorylated substrates by the ubiquitin system.

Substrate selection by Cdc4. The structure of the Skp1-Cdc4-CPD complex reveals the basis for phosphorylation-dependent recognition, the specificity of which is governed by three primary determinants. The substrate phospho-threonine is locked in place by direct contacts with three conserved and essential Arg residues. The preference for hydrophobic residues at the P-1 position (and perhaps P-2 position) is enforced by a hydrophobic pocket that lines the center of the WD40 propeller. Finally, the bias against basic residues at P+2 to P+5 is established by two conserved Arg residues positioned on the top of the propeller directly in-line with the axis of the bound peptide. These conclusions are supported by mutagenesis of key residues in Cdc4 and by structure-based engineering of Cdc4 to accept sub-optimal CPD sequences.

The construction of the Cdc4 phospho-peptide binding module differs from that of known phospho-Ser/Thr binding modules in an important respect. Known phospho-recognition domains, such as 14-3-3, WW and FHA domains appear to be composed of a series of dedicated interaction sites, each of which contributes incrementally to the overall binding interaction (Yaffe and Elia, 2001). The Cdc4-substrate interaction is dominated by extensively coordinated phospho-Thr and Pro residues, as well as by a striking positive electrostatic potential around the binding site. The hydrophobic pocket that selects residues in the P-2 and P-1 positions also contributes to binding affinity. In contrast to other phospho-recognition modules, however, the strong binding of the phosphorylated residue is partially offset by specific selection against basic residues in the substrate peptide, through electrostatic repulsion from a basic patch downstream of the phosphate binding pocket. These features allow the binding affinity for any given peptide to be precisely tuned. Thus, all of the natural CPD motifs in Sic1 are sub-optimal in one or more respects; indeed only peptides derived from the T45 site exhibit any detectable interaction with Cdc4 (Nash et al., 2001). These features

establish a requirement for substrate phosphorylation on multiple sites, which mediate a high affinity interaction in a manner that depends cooperatively on the number of phosphorylated residues.

In the case of wild type Sic1, at least six sites must be phosphorylated for high affinity binding by Cdc4. As shown here, mutation of the basic selection residues shifts the binding equilibrium to lower phosphorylated forms while in previous studies, it was demonstrated that introduction of a single optimal CPD into Sic1 causes premature Sic1 degradation and genome stability (Nash et al., 2001). An advantage of this system is that not only can the affinity of individual sites be tuned over a broad range, but the number and spacing of sites can be readily varied to establish a threshold for the targeting kinase. Thus Cdc4 is able to target numerous critical factors for phosphorylation-dependent degradation, including the Cdk inhibitor Sic1, the polarization factor Far1, the replication initiator Cdc6 and the transcription factor Gcn4, all of which may be controlled with different kinetics and different phosphorylation thresholds (Deshaies, 1999). These properties distinguish Cdc4 from other known phospho-peptide binding modules that typically interact with dedicated sites on their substrates through a single high affinity interaction (Pawson and Nash, 2000; Yaffe and Elia, 2001).

The mechanism that engenders a cooperative binding effect remains to be determined. In principle, multiple interactions sites might increase binding either by engaging more than one binding site on Cdc4, or by decreasing the probability of dissociation from Cdc4 (Deshaies and Ferrell, 2001; Harper, 2002; Nash et al., 2001). Cooperative interactions for the dual SH2 domain phosphatase SH-PTP2 and 14-3-3ζ rely on two substrate binding sites for high affinity recognition of bivalent ligands (Eck et al., 1996; Yaffe et al., 1997). Notably though, inspection of the WD40 surface does not reveal any other potential ligand binding pockets or grooves that might accommodate a phosphorylated peptide motif. Although secondary weak phospho-dependent interactions might occur, it is not obvious from the structure where such putative secondary sites might be located. In favor of the probabilistic cooperativity effect, mathematical modeling suggests that cooperative behaviour arises for the interaction between a single binding site and a polyvalent ligand as a function of the number of ligand sites. In effect multiple ligand sites increase the local concentration of ligand beyond a diffusion limited threshold for escape from the receptor. In the absence of candidate secondary sites, the simplest model is favored in which Cdc4 contains only a single phospho-dependent binding site.

Comparison to other phospho-peptide binding domains. The structure of the Cdc4 WD40 domain provides direct evidence that WD40-type repeats can assemble into propellers with more than seven blades (Fulop and Jones, 1999). One consequence of the additional blade is an enlarged channel through the center of the propeller, which creates a wide binding pocket that accommodates the core Leu-pThr-Pro ligand. This pocket contrasts to all other phospho-Ser/Thr binding domains, which engage their ligand through more shallow surface contacts within loops that extend from the core domain. WD40 domains are known to interact with other proteins in at least two different modes. In the Gb transducin and TUP1 WD40 domains, the protein interaction region occurs across the top of the propeller, much as in the case of Cdc4 (Sprague et al., 2000; Wall et al., 1995). In a second mode, defined for the WD40 domain of clathrin and the b-arrestin peptide, a "peptide-in-groove" interaction occurs on the bottom edge of the propeller

between the b-strands of the second blade (ter Haar et al., 2000). Modeling of b-TrCP, which binds the consensus motif DpSGXXpS [SEQ ID NO.42] in IkBa, b-catenin, and Vpu (Yaffe and Elia, 2001), suggests that an extensive basic region on the top of the propeller will engage substrate peptides in an analogous manner to Cdc4 .

Spatial orientation of SCF substrates. A conserved feature between all E3 structures solved to date is the large distance between the substrate binding site and the catalytic site (Huang et al., 1999; Zheng et al., 2002; Zheng et al., 2000). Modeling of the Skp1-Cdc4 complex onto a model of the Skp1-Cul1-Rbx1-E2 complex suggests that the substrate is positioned for direct frontal attack by the E2 catalytic site but that a gap of some about 65Å must be bridged between the two sites, presumably by the substrate polypeptide. Unexpectedly, superposition of the WD40 domain of Cdc4 with the LRR of Skp2 does not align the defined phosphopeptide binding pocket of Cdc4 with a potential phospho-recognition site of on the concave face of the LRR repeats (Zheng et al., 2002), at least as defined by mutational analysis of the related F-box protein Grr1 in yeast (Hsiung et al., 2001). If the relative position of substrates in the WD40 versus LRR class of F-box proteins differs, spatial plasticity in substrate presentation must be possible. This notion is consistent with the fact that the HIV protein Vpu is able to redirect the specificity of the F-box protein b-TrCP by bridging bTrCP to the host cell protein CD4, in a manner that depends on phospho-dependent recognition of Vpu by b-TrCP (Margottin et al., 1998). Similarly, it is possible to create synthetic adapters that bridge the substrate recognition site of an F-box protein to an ectopic substrate (Sakamoto et al., 2001). Finally, by definition all E3s must able to accommodate the substrate and the elongating ubiquitin chain generated by repeated catalytic cycles (Pickart, 2001). All of these points argue for considerable spatial leeway, and possibly flexibility of F-box protein orientations within the SCF catalytic cavity.

Based on the extensive Skp1-Skp2 interface, and on the inactivation of Cul1 by insertion of a flexible linker, it has been proposed that SCF complexes, and perhaps E3 enzymes in general, must present substrates to the catalytic site in a rigidly defined fashion (Zheng et al., 2002). However, the WD40 domain and the F-box of Cdc4 are linked only by a single α-helical stalk, with additional surface contact between the domains, all of which is mediated by non-conserved residues. It is thus somewhat difficult to reconcile the properties of the two F-box protein structures solved to date. Although it may be that regions truncated from Cdc4 to enable crystallization may normally help stabilize the interface, none of these regions are highly conserved between closely related Cdc4 family members. Perturbation of the rotational and translational position of the WD40 domain by introduction of additional residues into the stalk abrogates function in all cases, except for a long insertion of 12 residues. The fact that this gross structural change can be tolerated implies a degree of comformational plasticity with the catalytic cradle. This plasticity may facilitate the access of multiple ubiquitination sites within Sic1 to the catalytic center, as directed by the multiple low affinity CPD motifs in Sic1.

Insights into substrate recognition by human Cdc4. In metazoans, Cdc4 targets multiple critical regulators of cell division and development. Among these, cyclin E is a crucial substrate because its abundance must be strictly controlled in order to avoid precocious S phase entry and attendant genome instability (Spruck et al., 1999). Notably, it has been recently reported that mutational inactivation of hCDC4 occurs in several cancer cell lines that exhibit high

levels of cyclin E (Moberg et al., 2001; Strohmaier et al., 2001). In addition, hCDC4 may be mutated in up to 30% of endometrial cancers (Spruck et al., 2002). Quite strikingly, known cancer associated mutations in hCDC4 alter phosphoThr-binding residues. Given the probable requirement for homodimerization in active SCF complexes (Kominami et al., 1998; Suzuki et al., 2000), such mutations might be expected to acts in a partial dominant negative manner. Other critical substrates that appear to bind Cdc4 in a phosphorylation dependent manner include SEL-10, a negative regulator of the LIN-12/Notch pathway (Hubbard et al., 1997) that targets the transcriptionally active Notch intracellular domain for degradation (Gupta-Rossi et al., 2002; Wu et al., 2001) and the presenilins, dominant mutations in which predispose to familial early onset Alzheimer's disease (Selkoe, 2001; Wu et al., 1998). Mutations that interfere with hCdc4 activity may therefore compound multiple disease phenotypes.

Yeast and human Cdc4 exhibit a high degree of structural similarity, especially in the critical substrate binding region, and moreover, Cdc4 family members are functionally conserved since the hCdc4 substrate cyclin E is efficiently degraded in yeast in a CDC4-dependent manner (Koepp et al., 2001; Nash et al., 2001; Strohmaier et al., 2001). The structure of yeast Cdc4 thus affords insights for rational drug design. Significantly, the low affinity of individual natural CDP sites that engender the requirement for multisite phosphorylation means that even compounds of moderate affinity can readily out-compete the binding of fully phosphorylated substrates (Nash et al., 2001). Naively, inhibition of hCdc4-substrate interactions would be expected to exacerbate the deregulated proliferation caused by stabilization of cyclinE, Notch-IC or presenilin. However, if Cdc4 or Cdc4-like activities limiting for growth, Cdc4 antagonists may have heightened toxicity in cells that are hypomorphic for Cdc4 function. Alternatively, disruption of hCdc4 function may cause synthetic lethal effects in combination with otherwise non-lethal mutations in functionally overlapping pathways (Tong et al., 2001).

EXAMPLE 2

The following methods were used in the investigation described in the example:

Protein expression and purification. The Cdc4 fragment employed for crystallization was deleted for residues 1-262, 602-605, 609-624, and 745-779 to remove loop regions based on sequence alignments and limited proteolysis of the intact SCF^{Cdc4} complex. Skp1 was deleted for a non-conserved loop insertion spanning residues 37-64. A $^{GST}Skp1_{-}^{His6}Cdc4$ complex was co-expressed from plasmid pMT3169 in B934 (DE3) bacterial strain (Stratagene) cells grown in minimal media supplemented with a mixture of selenomethionine (40 μg/ml) and methionine (0.4ug/ml) and purified by double affinity tag chromatography (Nash et al., 2001). All mutations were constructed by standard methods using oligonucleotides listed in Table 7 and sequence verified in their entirety. Mutants were sub-cloned into pMT3055 or pMT3217 for expression in bacteria or yeast, respectively, as listed in Table 8. The WD40 domain of the helix α6 linker mutants Ala1, Ala2, Ala12, and helix α6 breaker could not be stably expressed in bacteria; the Ala12 mutant also could not be expressed in yeast.

Crystallization, data collection, structure determination and modeling. Hanging drops containing 1 μl of 20 mg/ml protein and 1.2 molar equivalents of the cyclin E derived CPD peptide (acetyl-Gly-Leu-Leu-pThr-Pro-Pro-Gln-Ser-Gly-amide) [SEQ ID NO 40]in buffer (10 mM HEPES pH 7.5, 250 mM NaCl, 1 mM DTT) were mixed with

equal volume of reservoir buffer (0.1 M Tris pH 8.5, 1.5 M ammonium sulphate). Crystals of the space group $P3_2$, (a =107.7Å, b = 107.7Å, c = 168.3Å, $\alpha = \gamma = 90°$, $\beta = 120°$), with two Cdc4–Skp1–CPD complexes in the asymmetric unit were obtained at 20°C. A Multiple Anomalous Dispersion (MAD) experiment was performed on a frozen crystal at the Advanced Photon Source (Argonne, IL) beamline BM 14-C and BM 14-D ($\lambda 1$ = 0.9798 Å, $\lambda 2$ = 0.9800 Å, $\lambda 3$ = 0.9000 Å) using a Quantum 4 ADSC CCD detector. Data processing and reduction were carried out with the HKL program suite (Otwinowski and Minor, 1997). The programs SHARP (de La Fortelle and Bricogne, 1997) and SnB (Miller et al., 1994) were used in combination to locate and refine 19 of the total 22 selenium sites. Following phasing and density modification, a model was built using O (Jones et al., 1991) and refined to 2.7 Å resolution with NCS restraints using CNS (Brunger et al., 1998) to a working R_{value} of 23.8% and R_{free} of 27.3%. Pertinent statistics for data collection and refinement are shown in Table 2. Amino acids 37-74, and 104-115 of Skp1 and amino acids 497-507 of Cdc4 were disordered and could not be modeled. 89.1% of the residues occupy the most favored regions of the Ramachandran plot, 10.8% the additional allowed region and 0.2% the generously allowed region.

Ribbons representations were generated using Ribbons (Carson, 1991), surface representations were generated using Grasp (Nicholls et al., 1991) and electron density maps were generated using O (Jones et al., 1991). A model of the ubiquitin–E2–SCF^{Cdc4}–CPD complex was generated by superposition of the Skp1 subunits of the Skp1–Cdc4–CPD structure and the Skp1–Cul1–Rbx1 structure (PDB ID 1LDK) (Zheng et al., 2002), the RING finger domains from Rbx1 in the same Skp1–Cul1–Rbx1 complex and from the Cbl subunit of the Cbl–UbcH7 structure (PDB ID 1FBV) (Zheng et al., 2000), and the E2 subunits of the Cbl–UbcH7 structure and an NMR-based Ubc1–ubiquitin model (PDB ID 1FXT) (Hamilton et al., 2001). The Skp1, RING domain and E2 subunits overlapped with RMSD values of 1.01 Å, 2.09 Å, and 2.04 Å respectively.

Cdc4 functional assays. *CDC4* mutant alleles were assessed for complementation of a *cdc4Δ* strain in a plasmid shuffle assay (Nash et al., 2001). Sensitivity to *SIC1* dosage was determined by transformation with pMT837 (*GAL1-SIC1*) or pMT767 (*GAL1-SIC1*^{T33V}) and plating on glucose medium or galactose medium. For in vitro capture of phospho-Sic1 by Cdc4, 0.5 µg of bacterially-expressed ^{HIS6}Sic1 was phosphorylated with immobilized Cln2–Cdc28 kinase from baculovirus-infected Sf9 cells and then incubated with 1 µg of immobilized wild type or mutant $Cdc4^{263-744}$–GST-Skp1, at 4°C for 1hr, washed 4 times and visualized by anti-Sic1 immunoblot. For isoelectric focusing (IEF)–2D gel analyses, an evenly distributed pool of phospho-Sic1 isoforms was generated by combining different time points in a Sic1 phosphorylation reaction. 2.5 µg of the phospho-Sic1 pool was bound to 5 µg of immobilized wild type or mutant $Cdc4^{1-744}$–GST-Skp1. Captured isoforms were separated by denaturing IEF–2D gel electrophoresis using pH3-10NL Immobiline gel strips (Amersham) and visualized by anti-Sic1 immunoblot. Alternatively, the pool of phospho-Sic1 isoforms was incubated in solution with a ubiquitination reaction mix containing ATP, ubiquitin, yeast E1, Cdc34 and either wild type or mutant SCF^{Cdc4} complex, composed of a 1:1 ratio of bacterial Cdc4–GST-Skp1 and insect cell-produced Cdc53–Rbx1, at 30°C for 1h as previously described (Nash et al., 2001).

Results

Alignment of Skp1 and Cdc4 homologs from various species and limited proteolysis of full length recombinant proteins were used to deduce loop regions in *Saccharomyces cerevisiae* Skp1 and Cdc4 that might interfere with protein crystallization (Figure 1). Crystals of a ternary complex of ScSkp1 bound to ScCdc4 and a CPD phosphopeptide were obtained that diffracted to a resolution of 2.7Å (Table 2). For Skp1, a non-essential loop spanning residues 37-64 was removed. The Cdc4 fragment used extends from residues 263 to 744, which encompasses the F-box motif to the end of the WD40 domain, and was engineered to remove two predicted loop regions (Figure 1B). This Cdc4 construct lacks an essential ~ 40 residue domain that precedes the F-box in different WD40 domain containing F-box protein family members (Wolf et al., 1999). The high affinity CPD phosphopeptide corresponds to nine residues of human cyclin E, Gly-Leu-Leu-pThr-Pro-Pro-Gln-Ser-Gly, [SEQ ID NO. 40] which binds Cdc4 with a K_d of 1 μM (Nash et al., 2001).

The F-box interface. Yeast Skp1 forms an elongated structure with a mixed α/β topology identical to that reported for human Skp1 (Schulman et al., 2000) and consists of a three-strand β sheet, denoted β1 to β3, and eight α-helices, denoted α1 to α8 (Figure 2A). The structure of Cdc4 consists of an F-box domain, an α-helical linker, and a WD40 domain (Figure 2A,B,C). The F-box domain is comprised of five α helices, denoted α0 to α4. This topology differs slightly from that reported for the F-box domain of hSkp2 , which consists of a loop region L1 and three helices denoted α1 to α3 (Schulman et al., 2000) Helix α0 in Cdc4 corresponds most closely in sequence and position to the loop region L1 of hSkp2 while a half turn remnant of Cdc4 helix α4 is discernable in the transition sequence between the hSkp2 F-box and the LRR domain. As observed in the hSkp1-hSkp2 complex, ScSkp1 and the F-box domain of Cdc4 associate by interdigitation of helixes α0 to α3 Cdc4 with helices α5 to α8 of Skp1, with the interface itself comprised of an inter-protein 4-helix bundle. This mode of association gives rise to a contiguous hydrophobic core that spans Skp1 and the F-box domain of Cdc4. Superposition of the yeast and human structures reveals that Skp1 helix α8 and F-box helix α4 deviate significantly in that only the first half of helix α8 is ordered in ScSkp1 and only a half turn fragment of the F-box helix α4 is apparent in hSkp2 (Figure 6A). The difference in position and length of F-box helix α4 and Skp1 helix α8 reflects the different roles these secondary structure elements play in the linkage between their respective F-box and ligand binding domains, as described below.

The WD40 domain. Eight copies of the WD40 repeat motif in Cdc4 form an 8 blade β-propeller structure (Figure 6B). The WD40 repeat motif of approximately 40 residues composes the outer β-strand of one propeller blade and the inner three strands of the adjacent blade in a continuous circular arrangement (Fulop and Jones, 1999). The actual Cdc4 structure contrasts to the 7 blade β-propeller predicted for Cdc4 and its orthologs based on previously solved WD40 domain structures, all of which contain only 7 blades (Koepp et al., 2001; Nash et al., 2001). This discrepancy is attributable to the cryptic nature of the 8th WD40 repeat motif. Structure based sequence alignment suggests that the WD40 domains of the F-box proteins Met30 and β-TRCP will form canonical 7-blade β-propeller structures (Figure 1B). A variant five β-strand structure occurs in blade 2, in which a large insert in the β12-β13 linker allows

the outermost $\beta 9^1$ strand to run parallel to the β9 strand. This five strand composition is unique to the fungal Cdc4 orthologs. In terms of overall structural dimensions, the WD40 domain resembles a conical frustum of 40Å diameter top surface and 50Å bottom surface, an overall thickness of 30Å and a central pore of 6Å diameter. The CPD binding site resides on the top surface of the frustum and runs across the edge of the pore, while the bottom surface of the frustum links to the F-box domain.

The F-box to WD40 domain linker. The F-box domain of Cdc4 is followed by a helical extension that forms a structured bridge to the WD40 domain. The bridge consists of two α-helices, α5 and α6, that together with helices α3 and α4 of the F-box domain form a platform and stalk-like structure that positions the WD40 domain well away from the F-box domain (Figure 2A,C). The relative orientation of the F-box domain and WD40 domain is imposed almost entirely through the integrity of the stalk-like helix α6, which is 30Å in length. The N-terminal end of helix α6 is anchored into the hydrophobic core of the F-box domain through interactions involving α6 residues Phe 355 and Leu 356 and F-box residues Ile 295, and Ile 296, Leu 315, Trp 316, and Leu 319 (Figure 2C). Helix α5 packs along side the base of helix α6 opposite to the F-box domain through hydrophobic interactions involving Tyr342, Leu 338 and Leu 334. The C-terminal end of helix α6 inserts obliquely between propeller blades α7 and α8 of the WD40 domain through van der Wals and hydrophobic interactions involving residues Trp 365 and Ile 361 with WD40 domain residues Val 687, Ile 696, Leu 726 and Phe 743 in βpropeller blades 7 and 8. Asn 364 of helix α6 also forms a tight hydrogen bond with the backbone carbonyl group of Phe 743 in propeller blade 8. The conservation of many of these residues, with the possible exception of those within helix α5, suggests that a structured linkage between the WD40 and F-box domains may be a common feature of the WD40 family F-box proteins.

The interdomain connection between the F-box and the WD40 domains of Cdc4 appears less rigidly structured than the corresponding region in hSkp2 (Figure 6A). Outside of the stalk helix α6, only two close contacts (< 3.5Å) are observed between the WD40 domain and other regions of Cdc4 (Figure 2C). These contacts consist of hydrogen bonds between Asn684 and Arg700 in two loop regions of propeller blade 7 with Glu 323 in the α4–α5 linker of the helical extension. Both hydrogen bonds are maintained in the two Cdc4 molecules of the crystal asymmetric unit but all three residues are poorly conserved amongst Cdc4 orthologues (Figure 1B). The lack of additional stabilizing interactions suggests that the F-box to WD40 domain linker is not exceedingly rigid, and indeed, the WD40 domain in the two Cdc4 molecules of the crystal asymmetric unit differ relative to their F-box domains by a 5° rotation about the long axis of helix α6. In contrast, in hSkp2 the F-box domain helix α4 terminates abruptly in an immediate transition to the LRR domain fold such that the adjoined domains form a rigid hydrophobic core (Schulman et al., 2000). Although the Skp2 and Cdc4 families of F-box proteins employ structurally divergent F-box interfaces, the general position of the WD40 and LLR domains are nonetheless similar (Figure 6A).

Model of the SCF^{Cdc4} E2 complex. The structure of the Skp1-Cdc4-CPD complex sheds light on how substrates are presented by the F-box protein to the E2 for ubiquitin transfer. A complete model of the E2–SCF^{Cdc4}–substrate complex consisting of ubiquitin, hUbc7, hCul1, hRbx1, ScCdc4, ScSkp1, and the CPD peptide is shown in Figure 6B.

This model is based on the reconstructed E2–SCF^{Skp2} complex derived by Pavletich and colleagues (Zheng et al., 2002), in conjunction with an NMR-based ubiquitin–E2 thioester model (Hamilton et al., 2001). Two interesting features are apparent. First, the distance between the E2 active site cysteine and the phosphate group of the bound CPD peptide is approximately 59 Å, which is similar to the spacing reported between the substrate interaction site and the E3 catalytic site in the hUbc7–Cbl structure (Zheng et al., 2000). Secondly, the WD40 domain presents the CPD peptide in a direct line-of-sight to the E2. Although the ligand-binding site on hSkp2 has not been determined, mutagenesis studies on the LRR-containing F-box protein Grr1 in yeast suggest that substrates bind to the inner side of the curved repeat surface (Hsiung et al., 2001). If the position of this site is maintained in hSkp2, then the LRR domain of Skp2 is predicted to project substrates in an orthogonal direction to that of the Cdc4 WD40 domain (Figure 6A).

Phosphopeptide recognition. The CPD binding surface represents the most conserved part of the WD40 repeat domain structure (Figure 7A-D). The central CPD sequence Leu-pThr-Pro-Pro [SEQ ID NO. 41] was modeled unambiguously in unbiased experimental electron density maps in both Skp1–Cdc4–CPD complexes of the crystal asymmetric unit (Figure 3). Interpretable electron density is also apparent for the P-2 Leu, P+3 Gln, P+4 Ser, and P+5 Gly positions, but only in one complex of the crystal asymmetric unit. The CPD peptide binds in an extended manner across β-propeller blade 2 with the N-terminus oriented towards the central pore of the WD40 domain and the C-terminus oriented towards the outer rim. Identical substrate peptide orientations and contacts were observed for an independent Skp1-Cdc4-CPD structure with a phosphopeptide derived from the transcription factor Gcn4, which is a physiological substrate of Cdc4 in yeast (Meimoun et al., 2000; Chi et al., 2001). However, of the Gcn4 peptide sequence, Phe-Leu-Pro-pThr-Pro-Val-Leu-Glu-Asp [SEQ ID NO. 43], only the core residues Pro-pThr-Pro had discernable electron density.

The CPD sequence requirements for the CPD-Cdc4 interaction are fully accounted for by structural elements in the WD40 domain. An absolute requirement for phosphorylation at Ser or Thr at the P-0 position of the CPD derives from a network of electrostatic interactions and hydrogen bonds that coordinate the P0 pThr phosphate group (Figure 7C, D). This interaction is mediated by residues that are conserved across all Cdc4 orthologs (Figure 1B). The P0 phosphate group forms direct electrostatic interactions with the guanidinium groups of Arg485, Arg467, and Arg534 and a direct hydrogen bond with the side chain of Tyr548. The side chain of Tyr548 is coordinated by stacking interactions with the guanidinium group of Arg572, which in turn is coordinated by a hydrogen bond to the side chain of Tyr574. Although Cdc4 shows a 6-fold preference for pThr over pSer (Nash et al., 2001), the structural basis for this selectivity is not obvious since the Cγ methyl group of Thr is directed towards solvent and does not make contact with the WD40 domain surface.

A second absolute requirement for CPD–Cdc4 interaction rests on the P+1 proline, the side chain of which projects into a three-sided pocket on the WD40 surface. One side of this pocket is formed by the side chain of Trp 426, which packs in a coplanar manner with the P+1 proline side chain. The opposite side of this binding pocket is formed by the side chain of Arg 485 via coordination of the proline side chain and backbone carbonyl group through

van der Waals and hydrogen bonding interactions, respectively. The side chains of Thr 441 and Thr 465 define the remaining side of the P+1 proline binding pocket, with Cγ side chain groups composing a hydrophobic surface. The hydroxyl groups of Thr 441 and 465 orient away from the P+1 binding pocket, where they are well placed to influence binding specificity for CPD residues C-terminal to the P+1 position. Unlike Trp 426 and Arg 485, which are invariant amongst the Cdc4 orthologs, Thr 441 and Thr 465 are both substituted with Ile in the *S. pombe* Cdc4 ortholog Pop1 (Figure 1B). This substitution might restrict CPD sequences able to bind Pop1 through steric or hydrophobic constraints on residues C-terminal to the P+1 proline position.

Cdc4 displays a strong preference for the hydrophobic residues Leu/Ile/Pro at the P-1 and Leu/Ile at the P-2 CPD positions. In the crystal structure, the P-1 Leucine side-chain fits into a hydrophobic pocket composed of invariant residues Trp 426, Trp 717, and Thr 386, and the conserved hydrophobic residue Val 384. While less precisely modeled, the main chain position of Leu -2 lies in close proximity to a third hydrophobic pocket composed of the invariant residue Tyr574, and the conserved hydrophobic residues Met 590 and Leu634. The hydrophobic character of the P-1 and P-2 pockets is manifest as selection against both charged and small polar residues at these positions in the CPD consensus (Nash et al., 2001).

The WD40 phospho-recognition domain of Cdc4 is unusual in that it exhibits strong selectivity against either Arg or Lys residues in the P+2 to P+5 CPD positions, but otherwise shows no sequence preference at these positions (Nash et al., 2001). In the crystal structure, the side chain of P+2 Pro is directed towards solvent, while the main chain conformation of Pro+1 and Pro+2 causes the CPD to kink away from the peptide-binding surface from the Pro+2 position onward. As a result, only one additional contact with Cdc4 is made by the CPD following the Pro +1 position, namely a weak hydrogen bond with sub-optimal geometry between the P+4 Gln side chain and the side chain of Arg 485. Because the P+1 Pro main chain is forced away from the WD40 domain surface, the selection against basic residues in the P+2, +3, +4 and + 5 positions in the CPD consensus is almost certainly due to through-space electrostatic repulsion. This effect arises from a dominant positive electrostatic potential generated by both the invariant triad of Arg residues that comprise the core pThr-Pro binding pocket, and by a radial extension of the surface due to Arg 572, Arg 443 and Lys 402, the former two of which are conserved amongst Cdc4 orthologs (Figure 7B).

A number of natural mutations detected in metazoan orthologs of Cdc4 corroborate the structure-based analysis. Two ovarian cancer cell lines bear missense mutations at conserved Arg residues that correspond to Arg 467 and Arg 534 in yeast Cdc4 (Moberg et al., 2001). In the crystal structure, these residues make direct contact with the P0 phosphate group and are essential for function (Figure 7 C, D). In a recent study of human primary endometrial tumors, mutations in phosphate-binding Arg residues equivalent to Arg 467 and Arg 485 were detected in 2 of 13 tumor samples (Spruck et al., 2002). Other cancer-associated nonsense and frameshift mutations truncate hCdc4 within the WD40 domain (Moberg et al., 2001; Strohmaier et al., 2001; Spruck et al., 2002). Similarly, all three characterized mutations in the Drosophila *ago* gene that lead to excess cell proliferation affect the WD40 domain (Moberg et al., 2001). One of these mutations, Ala1118Val, corresponding to position Ser532 in ScCdc4 substitutes a conserved small residue with a bulkier residue at the center of the critical Arg 434-Arg467-Arg534 triad (Figure 7C).

Mutational analysis of the F-box to WD40 domain linker. To probe the importance of orientation and rigidity in the F-box WD40 inter-domain linker, point mutations, insertions or deletions were introduced into the platform and stalk structure of Cdc4. None of these deletions affected the ability of the recombinant proteins to bind phospho-Sic1 *in vitro* or protein abundance in vivo (Figure 8A and data not shown). Introduction of the helix destabilizing residues glycine and proline into helix α5 did not compromise Cdc4 function in vivo (Figure 8B), consistent with the poorly conserved nature of this region (Figure 1B). However, two different deletions of helix α5 eliminated Cdc4 function in vivo, indicating that the F-box–WD40 domain interface is an essential structural component. Similarly, placement of helix destabilizing residues at the center of helix α6 or the lengthening of this helix by the insertion of one, two, three, four, 8 or 12 amino acid residues disrupted Cdc4 function in vivo. Helix α6 is thus critical for productive orientation of the WD40 domain.

Mutational analysis of the CPD binding surface. Previous mutational analysis based on sequence conservation in the Cdc4 family identified Arg467, Arg485 and Arg534 as essential for substrate binding and function in yeast (Nash et al., 2001). Two of the three corresponding residues in hCdc4, Arg 417 and Arg 457, are essential for the binding of phospho-cyclin E, while the third corresponding to Arg485 was not tested (Koepp et al., 2001). To systematically probe the role of residues that form the highly conserved peptide binding surface, a panel of Cdc4 mutants was generated and each were tested for pSic1 binding in vitro, complementation of a *cdc4Δ* strain and sensitivity to increased *SIC1* dosage. Four mutants, Arg467Ala, Arg485Ala, Arg534Ala, and Trp426Ala were unable to bind phospho-Sic1 in vitro or complement a *cdc4Δ* strain, but were fully competent for Skp1 binding (Figure 8A, B). The essential function of these residues is not confined to elimination of Sic1 because none of the corresponding mutant alleles were able to rescue a *cdc4Δ sic1Δ* strain. These results reflect the critical structural role played by these residues in coordination of the P0 phosphate and the P+1 proline of the CPD. Mutation of the remaining phosphate-coordinating residue, Tyr548, did not cause loss of viability but did result in dosage sensitivity to $SIC^{Thr33Val}$, which encodes a partially stabilized version of Sic1 (Figure 8C). Mutation of Arg 572 had the same effect, as befits the observed stacking interaction between this residue and Tyr 548. Although both mutants were severely impaired for binding to phospho-Sic1 in vitro, this effect may be exacerbated by the tendency of these recombinant proteins to aggregate. In summary, the six residues that directly or indirectly coordinate the primary pThr-Pro core motif are critical for CPD recognition in vitro and Cdc4 function in vivo.

Disruption of residues that confer selection at the P-2, P-1 and P+2 to P+5 positions had only modest effects on the ability of Cdc4 to target pSic1. A Trp717Asn mutation predicted to disrupt the P-1 pocket conferred sensitivity to dosage of $SIC1^{Thr33Val}$, but did not overtly affect the pSic1-Cdc4 interaction in vitro. Individual mutations in all other residues that are well positioned to affect substrate selection, namely Arg443Ala, Arg443Asp, Lys402Ala, Tyr574Phe and Val384Asn were indistinguishable from wild type in each of the assays used. Substrate selection residues on the WD40 surface thus contribute only modestly if at all to the essential function of Cdc4. As described below, however, these residues play a subtle but critical role in setting the phosphorylation threshold for the CPD-Cdc4 interaction.

Modulation of CPD substrate selectivity. A critical feature of the Sic1-Cdc4 interaction is the requirement for phosphorylation of Sic1 on multiple sites. To enforce this requirement, each of the phosphorylation sites in the native Sic1 sequence are sub-optimal in one or more respects (Figure 9A). The Cdc4-CPD structure suggests that selectivity against basic residues may be due to electrostatic repulsion generated from the conserved patch of basic residues in and around the CPD binding pocket, while selection for hydrophobic residues arises from the P-1 pocket that is composed in part by Val 384 and Trp717. To examine the basis for selection against sub-optimal CPD motifs, the effects of mutations in non-essential residues in these two regions on the multisite phosphorylation requirement for Sic1 recognition were assessed.

The ability of Cdc4 to capture various phosphoisoforms of wild type Sic1 from a pool of recombinant Sic1 that had been phosphorylated to various extents by Cln2-Cdc28 was monitored. As resolved by isoelectric focusing, this pool contained roughly equal amounts of Sic1 phosphorylated on 1, 2, 3, 4, 5, 6, 7, 8 and 9 sites. Wild type Cdc4 was only able to capture Sic1 phosphorylated on six or more sites (Figure 9B). This result formally demonstrates the transition in binding affinity between 5 and 6 phosphorylation sites, as initially inferred from capture of a series of Sic1 phosphorylation site mutants by Cdc4 (Nash et al., 2001). The role of positive electrostatic potential in selecting against sub-optimal CPD sequences with basic residues at C-terminal positions was tested with the Lys402Ala Arg443Asp double mutant. This mutant was able to select Sic1 phosphoisoforms that contained as few as three phosphorylation sites (Figure 9B). The ability of the Lys402Ala Arg443Asp double mutant to capture lower phosphorylated forms of Sic1 is also evident in one-dimensional SDS-PAGE (Figure 8A). Similarly, perturbation of the P-1 hydrophobic pocket with a Val384Asn Trp717Asn double mutation allowed capture of Sic1 phosphorylated on as few as four sites. These in vitro binding results were recapitulated in solution-based in vitro ubiquitination assays with wild type and mutant forms of Cdc4. Both double mutant forms of Cdc4 were able to convert Sic1 phosphoryated on four or five sites to oligo-ubiquitinated species, whereas wild type Cdc4 was unable to do so (Figure 9C). The double mutants were, however, less efficient than wild type at elaborating fully ubiquitinated species of phospho-Sic1, perhaps because of protein stability effects or interference with catalytic steps after substrate binding. This interpretation is consistent with the sensitivity of strains bearing the double mutant alleles to $SIC1^{Thr33Val}$ dosage (Figure 8B). Overall, re-engineering of negative selection residues in the Cdc4 WD40 domain supports the notion that the series of sub-optimal CPD motifs in Sic1 sets a high phosphorylation threshold for its recognition by Cdc4.

Discussion

The structure of the Skp1-Cdc4-CPD complex provides direct visualization of substrate orientation within an SCF complex. Insights gained from the structure include the unexpectedly frail interface between the F-box and the WD40 repeat domain, the basis for dedicated pThr-Pro dipeptide recognition by a novel eight-blade WD40 propeller, and a detailed understanding of the basis for selection against natural CPD sequences. The latter feature appears to be tailored to enforce multisite phosphorylation dependent degradation of Sic1, which in turn would help engender a highly cooperative onset of DNA replication (Nash et al., 2001). Similar principles may well operate for other Cdc4 substrates, including cyclin E, $Notch^{IC}$ and presenilin in mammalian cells (Strohmaier et al., 2001; Lai, 2002; Selkoe,

2001). Because yeast and human Cdc4 are structurally and functionally analogous (Nash et al., 2001; Strohmaier et al., 2001; Koepp et al., 2001), the structure of yeast Cdc4 affords obvious insights for pharmacological modulation of hCdc4 function in these pathways. Interestingly, a significant proportion of characterized human and fly *CDC4* mutations alter residues in the CPD binding pocket. Given the probable requirement for homodimerization in active SCF complexes (Wolf et al., 1999), such mutations might act in a partial dominant negative manner to confer a growth advantage in the heterozygous state.

Phospho-recognition by Cdc4. The specificity of phosphorylation-dependent recognition by the WD40 domain of Cdc4 is governed by three main determinants: (i) a dedicated pThr-Pro binding pocket; (ii) a deep hydrophobic pocket that selects hydrophobic residues N-terminal to the phosphorylation site, and (iii) a through space electrostatic selection against basic residues C-terminal to the phosphorylation site. As for all documented phospho-dependent lipid/protein recognition modules, the Cdc4 WD40 domain employs arginine residues to directly contact the phosphate group of the ligand. However, unlike most domains in which adjacent residues impose subtle effects on specificity (Yaffe and Elia, 2001), the P+1 proline is an integral component of the core binding determinant (Nash et al., 2001). In the Cdc4-CPD co-crystal, ligand residues are locked in place by direct contact of the phosphate and proline carbonyl groups with three conserved and essential Arg residues, while the proline side chain inserts into a tight hydrophobic pocket formed by Trp426, Thr441, and Thr465. Because the phospho-binding pocket infrastructure has no obvious demarcation between the pThr and Pro binding sites, the Cdc4 WD40 domain is in effect a dedicated pThr-Pro binding module.

Comparison to other peptide recognition modules. Interesting parallels can be drawn between the Cdc4 WD40 domain, 14-3-3 domains and the class IV WW domains, which all have the ability to recognize phospho-Ser/Thr epitopes in the context of adjacent proline residues (Yaffe and Elia, 2001). The interaction of the Pin1 class IV WW domain with a pSer-Pro peptide differs from Cdc4 in that it does not rely on an extensive network of Arg residues for phosphate coordination (Verdecia et al., 2000). However, a striking similarity between Pin1 and Cdc4 lies in the P+1 proline binding pocket, which in both cases depend on a highly conserved tryptophan side chain to engage the P+1 proline pyrrolidine ring through a coplanar interaction. In contrast to Cdc4, Pin1 actually displays a preference for Arg in the P+2 position, such that the binding specificity of the pSer-Pro recognition domain closely matches that of the targeting CDK enzymes.

14-3-3 domains bind pSer epitopes with a preference, but not an absolute requirement, for proline residues at the P+2 position (Yaffe et al., 1997). This less stringent selection arises because the 14-3-3 proline binding pocket is able to accommodate other residues with propensity to form β-turns. Interestingly, the proline preferences in both the 14-3-3 and Cdc4 WD40 domains give rise to the same qualitative effect: in each case the prolines terminate direct interactions between the peptide and the ligand binding domain by orienting the peptide away from the domain surface. In the case of Cdc4, biologically significant electrostatic effects operate in spite of the loss of direct peptide contact. Physiologically relevant substrate anti-selection mediated by charge repulsion is unique amongst known protein interaction modules.

The structure of the Cdc4 WD40 domain provides direct evidence that WD40-type repeats can assemble into propellers with more than seven blades (Fulop and Jones, 1999). WD40 domains are known to interact with other proteins in at least two different modes, either across the front face of the propeller, as in the case of Cdc4, or on the outer edge of the propeller as in the case of clathrin (ter Haar et al., 2000). Modeling of the F-box protein β-TrCP, which binds the doubly phosphorylated consensus motif DpSGXXpS [SEQ ID NO. 42] in IκBα, β-catenin, and Vpu (Yaffe and Elia, 2001), reveals an extensive conserved basic region on the front face of the propeller, which may engage substrate phosphoepitopes in an analogous manner to Cdc4.

Spatial orientation of SCF substrates. A conserved feature between all E3 structures solved to date is the substantial distance between the substrate binding site and the catalytic site (Huang et al., 1999; Zheng et al., 2000; Zheng et al., 2002). Superposition of the Skp1-Cdc4 complex onto a model of the Skp1-Cul1-Rbx1-E2-ubiquitin complex suggests that the substrate is positioned for direct frontal attack by the E2 catalytic site, but that a gap of some 59Å between the two sites must be bridged, presumably by the substrate polypeptide. The disordered structure of Sic1 lends itself to this possibility (Nash et al., 2001). Intriguingly, overlay of the WD40 domain of Cdc4 with the LRR of Skp2 does not align the defined phosphopeptide binding pocket of Cdc4 with a potential phospho-recognition site on the concave face of the LRR repeats (Zheng et al., 2002), at least as defined by mutational analysis of the related F-box protein Grr1 in yeast (Hsiung et al., 2001). If the relative position of substrates in the WD40 versus LRR class of F-box proteins do in fact differ, spatial leeway in substrate presentation must be possible.

Based on the extensive Skp1-Skp2 interface, and on the inactivation of Cul1 by insertion of a flexible linker, it has been proposed that SCF complexes, and perhaps E3 enzymes in general, must present substrates to the catalytic site in a rigidly defined fashion (Zheng et al., 2002). Unexpectedly, the WD40 domain and the F-box of Cdc4 are linked only by a single α-helical stalk, with very limited additional contacts. Despite the lack of sequence conservation in the α helix 6 structure that supports the WD40 domain, spatial constraints are nevertheless evident, as shown by the sensitivity of the structure to rotational and translational shifts caused by insertion of additional residues into the stalk. It is also possible that regions truncated from Cdc4 to enable crystallization may normally help stabilize the inter-domain interface.

Cooperativity in substrate selection by Cdc4. The properties of the Cdc4 phosphopeptide binding module differ from those of other known modules in the important respect that the interaction with core recognition elements is partially offset by specific selection against basic residues in the substrate peptide. This feature establishes an intrinsic antagonism between the recognition mechanism and the targeting CDK kinases, which prefer Ser/Thr-Pro sites with C-terminal basic residues (Endicott et al., 1999). Significantly, all of the natural CPD motifs in Sic1 contain one or more mismatches to the optimal CPD consensus. This system based on positive and negative ligand selection may not only set an elevated threshold for kinase activity, but may also allow the threshold to be precisely tuned for any given substrate by varying the number, spacing and properties of each site. Thus, Cdc4 is able to target numerous critical factors for phosphorylation-dependent degradation, including the Cdk inhibitor Sic1, the CDK inhibitor and polarization factor Far1, the replication initiator Cdc6 and the transcription factor Gcn4, all of which may be

controlled with different kinetics and different phosphorylation thresholds (Patton et al., 1998). In one extreme, typified by Gcn4 and cyclin E, the substrate may contain a high affinity site that is augmented by several minor low affinity sites (Meimoun et al., 2000; Chi et al., 2001; Strohmaier et al., 2001). In the other, more akin to Sic1, a large number of weak sites may cooperate to drive high affinity binding only when a phosphorylation threshold is reached. As shown here, mutation of either the distal basic selection region or the P-1 pocket in Cdc4 shifts the binding equilibrium to lower phosphorylated forms of Sic1, which, in the absence of other structural effects that may compromise Cdc4, would be predicted to cause premature DNA replication and genome stability (Nash et al., 2001). These features distinguish Cdc4 from other known phospho-peptide binding modules characterized to date that typically interact with dedicated sites on their substrates through a single high affinity interaction.

The mechanism that underlies the cooperative binding transition of the phospho-Sic1–Cdc4 interaction between five and six phosphorylation sites remains to be determined. In principle, multiple interactions sites might increase binding by engaging more than one binding site on Cdc4 (Figure 9D). This type of cooperative interaction is common in biological systems, as in the avidity of antibodies for polyvalent ligands and pathogen-host interactions (Mammen et al., 1998). Analogous cooperative binding interactions occur in signaling pathways. For instance, the dual SH2 domain phosphatase SH-PTP2 and the 14-3-3ζ protein both engage two substrate binding sites on their respective ligands (Eck et al., 1996; Yaffe et al., 1997). However, inspection of the Cdc4 WD40 domain surface does not reveal any obvious ligand binding sites that might accommodate a second phosphorylated peptide motif, nor is there any biochemical evidence for secondary binding sites (Nash et al., 2001). In addition, the wide range of substrates and site spacing accommodated by Cdc4, including random concatamers of synthetic CPD sites (Nash et al., 2001), is a priori difficult to explain by two or more fixed binding sites on Cdc4.

Instead, a model is favored that requires only a single phospho-dependent binding site on Cdc4 (Figure 9D). In this scheme, phosphorylation of multiple CPD sites on Sic1 increases the local concentration of sites around Cdc4 once the first CPD site is bound, to the point where diffusion limited escape from the receptor is overwhelmed by the probability of re-binding of any one CPD site. In a sense, Sic1 becomes kinetically trapped in close proximity to Cdc4. Mathematical modeling of an idealized polyvalent ligand-monovalent receptor interaction indicates that the rate of ligand escape from the receptor exhibits a negative exponential dependence on the number of ligand sites. The term allovalent is proposed to describe the ability of multiple weak spatially separated ligand sites to cooperatively interact with a single receptor site. The prevalence of multisite phosphorylation (Cohen, 2000), and indeed of polyvalent ligands in general (Mammen et al., 1998), suggests that this type of behavior may underlie many biological processes.

The present invention is not to be limited in scope by the specific embodiments described herein, since such embodiments are intended as but single illustrations of one aspect of the invention and any functionally equivalent embodiments are within the scope of this invention. Indeed, various modifications of the invention in addition to those shown and described herein will become apparent to those skilled in the art from the foregoing description and accompanying drawings. Such modifications are intended to fall within the scope of the appended claims. In particular

it will be appreciated that the references to specific amino acid residues for particular a SCF complexes, and components thereof (e.g. F-box protein) illustrated in the Tables and Figures, in no way limits the scope of the invention and it will be appreciated that a person skilled in the art could determine the specific corresponding amino acid residues for other SCF complexes and components thereof.

All publications, patents and patent applications referred to herein are incorporated by reference in their entirety to the same extent as if each individual publication, patent or patent application was specifically and individually indicated to be incorporated by reference in its entirety. All publications, patents and patent applications mentioned herein are incorporated herein by reference for the purpose of describing and disclosing the cell lines, vectors, methodologies etc. which are reported therein which might be used in connection with the invention. Nothing herein is to be construed as an admission that the invention is not entitled to antedate such disclosure by virtue of prior invention.

It must be noted that as used herein and in the appended claims, the singular forms "a", "an", and "the" include plural reference unless the context clearly dictates otherwise. Thus, for example, reference to "a host cell" includes a plurality of such host cells, reference to the "antibody" is a reference to one or more antibodies and equivalents thereof known to those skilled in the art, and so forth.

Table 1.

Data Collection, Structure Determination, and Refinement Statistics

	Peak	Inflection	Remote
Wavelength (Å)	0.9798	0.9800	0.9000
Resolution (Å)	2.8	2.9	2.7
R_{sym} (%)	5.9 (38.7)	6.1 (36.1)	5.0 (28.9)
Total Reflections	311509	187010	298371
Unique Reflections	107167	96027	116218
Completeness (%)	99.8 (99.1)	99.3 (98.3)	97.7 (93.6)
I/σ	9.9 (2.7)	7.4 (2.1)	10.1 (2.9)
Phasing Power			

Refinement statistics	
Resolution range (Å)	20-2.8
Reflections	103863
R_{factor}/R_{free} (%)	24.09/28.71
Rms deviations	
Bonds (Å)	0.0091
Angles (°)	1.3453

Space group $P3_2$: a = b = 107.7 Å, c = 168.3 Å; a = b = 90° , c = 120° ;
Two molecules per asymmetric unit.

[1]Data for the highest resolution shell (2.90-2.80 Å)

[2]Rsym = 100 x $\Sigma|I - \langle I\rangle|/\Sigma\langle I\rangle$, where I is the observed intensity and <I> is the average intensity from multiple observations of symmetry-related reflections.

[3]Phasing power for isomorphous and anomalous acentric reflections, where phasing power = $\langle(|F_{h,c}| /$ phase-integrated lack of closure)>.

[4]R_{free} was calculated with 8.8% of the data.

Table 2.
Data Collection, Structure Determination, and Refinement Statistics

Phasing Statistics	Peak	Inflection	Remote
Wavelength (Å)	0.9798	0.9800	0.9000
Resolution (Å)	2.8 (2.9-2.8)	2.9 (3.0-2.9)	2.7 (2.8-2.7)
R_{sym} (%)	5.9 (37.2)	6.1 (36.1)	5.0 (28.9)
Total Reflections	311509	187010	298371
Unique Reflections	107167	96027	116218
Completeness (%)	99.8 (99.1)	99.3 (98.3)	97.7 (93.6)
I/σ	9.9 (2.7)	7.4 (2.1)	10.1 (2.9)
Phasing Power (ISO/ANO)	5.2/1.3	4.0/0.94	0/0.91

Refinement statistics (remote wavelength)

Resolution range (Å)	20-2.7	# protein atoms	9364
Reflections	113960	# water molecules	72
R_{factor}/R_{free} (%)	23.8/27.3		
Rms deviations			
Bonds (Å)	0.0089		
Angles (°)	1.42		

Space group $P3_2$: a = b = 107.7 Å, c = 168.3 Å; a = b = 90°, c = 120°
Two Skp1-Cdc4-CPD complexes per asymmetric unit

Numbers given in parantheses refer to data for the highest resolution shell.
[1]Rsym = 100 x $\Sigma|I - \langle I\rangle|/\Sigma\langle I\rangle$, where I is the observed intensity and <I> is the average intensity from multiple observations of symmetry-related reflections.
[2]Phasing power for isomorphous and anomalous acentric reflections, = $\langle[|F_h(calc)/\text{phase-integrated lack of closure}]\rangle$.
[3]R_{free} was calculated with 8.8% of the data.

Table 3.
Atomic Contacts of a Substrate Binding Pocket

No. of Atomic Interaction	CDC4 WD40 Motif Atomic Contact	CDC4 atomic Contact	CPD Motif Atomic Contact
1	Ile 295 Ile296 Leu 315 Trp 316 Leu 319	Phe 255 Leu356	
2	Val 687 Ile 696 Leu 726 Phe 743	Trp 365 Ile 364	
3	Phe 743	Asn 364	
4	Asn 684 Arg 700	Glu 323	
5	Arg 485 Arg 467 Arg 534 Tyr 548		PO pTyr Phosphate
6	Trp 426 Arg 485 Thr 386 Thr 441 Thr 465		P+1 Proline side chain
7	Trp 426 Trp 717 Thr 386 Val 384		P+1 Leucine side chain
8	Tyr 574 Thr 386 Val 384		Leucine +2

Table 4.
Atomic Contacts of a Substrate Binding Pocket

No. of Atomic Interaction	CDC4 WD40 Motif/F-box Domain Atomic Contact	CDC4 atomic Contact	CPD Motif Atomic Contact	Atomic Interaction Property
1	Ile 295 Ile296 Leu 315 Trp 316 Leu 319	Phe 355 Leu356		hydrophobic interactions and van der Wals interactions
2	Val 687 Ile 696 Leu 726 Phe 743	Trp 365 Ile 361		van der Wals and hydrophobic interactions
3	Phe 743	Asn 364		hydrogen bond
4	Asn 684 Arg 700	Glu 323		hydrogen bonds
5	Arg 485 Arg 467 Arg 534 Tyr 548		PO pTyr or pSer Phosphate at P-O position of CPD	electrostatic interactions hydrogen bond
6	Trp 426 Arg 485 Thr 441 Thr 465		P+1 Proline side chain and backbone carbonyl of CPD	hydrogen and van der Wals hydrophobic interations
7	Trp 426 Trp 717 Thr 386 Val 384		P-1 Leucine (or Ile/Pro) side chain	hydrophobic interactions
8	Tyr 574 Met 590 Leu 634		Leucine –2 Leu/Ile at P-2 position	hydrophobic interactions
9.	Tyr 342 Leu 338 Leu 334			hydrophobic interactions

Table 5

Determinants of pThr-Pro binding

	P-Sic1 pull down	gal Sic1wt	gal Sic1T45A	gal Sic1T33V	gal Sic1-7	gal Sic1-6	gal Sic1-5	gal Sic1-4	gal Sic1-3	shuffle
WT	bind	alive	dead	alive						alive
~~R374A~~	~~NA~~									~~alive~~
R443A	bind	alive	dead	alive						alive
~~R446A~~	~~NA~~									~~alive~~
R467A	no bind									dead
R485A	no bind									dead
R534A	no bind									dead
R572A	no bind	alive	dead	dead						alive
~~R655A~~	~~NA~~									~~alive~~
W426A	no bind									dead
V384N	bind	alive	dead	alive						alive
K402A	bind	alive	dead	alive						alive
R443D	bind	alive	dead	alive						alive
Y548F	no bind	alive	dead	dead						alive
Y574F	bind	alive	dead	alive						alive
W717N	bind	alive	dead	dead						alive
T441I/T465I	(in progress)									(in progress)
K402A/R443D	bind	alive	dead	dead						alive
W717N/V384N	bind	alive	dead	dead						alive
quad	(in progress)									dead

Table 6

```
REMARK peptide link removed (applied DPEP): from A    31   to A    45
REMARK peptide link removed (applied DPEP): from A    73   to A    86
REMARK peptide link removed (applied DPEP): from B    496  to B    508
REMARK peptide link removed (applied DPEP): from C    31   to C    45
REMARK peptide link removed (applied DPEP): from C    73   to C    86
REMARK peptide link removed (applied DPEP): from D    496  to D    508
REMARK peptide link removed (applied DPPP): from E    4    to E    5
REMARK coordinates from minimization and B-factor refinement
REMARK refinement resolution: 20 - 2.8 A
REMARK starting r= 0.2415 free_r= 0.2846
REMARK final    r= 0.2409 free_r= 0.2871
REMARK rmsd bonds= 0.009114  rmsd angles=  1.34531
REMARK B rmsd for bonded mainchain atoms=  1.230  target= 1.5
REMARK B rmsd for bonded sidechain atoms=  1.778  target= 2.0
REMARK B rmsd for angle mainchain atoms=  2.103  target= 2.0
REMARK B rmsd for angle sidechain atoms=  2.675  target= 2.5
REMARK target= mlf  final wa= 2.77695
REMARK final rweight=  0.1078 (with wa= 2.77695)
REMARK md-method= torsion  annealing schedule= constant
REMARK starting temperature= 2000  total md steps= 1 * 100
REMARK cycles= 2 coordinate steps= 20 B-factor steps= 10
REMARK sg= P3(2) a= 107.669 b= 107.669 c= 168.3 alpha= 90 beta= 90 gamma= 120
REMARK topology file 1  : CNS_TOPPAR:protein.top
REMARK topology file 2  : CNS_TOPPAR:dna-rna.top
REMARK topology file 3  : CNS_TOPPAR:water.top
REMARK topology file 4  : CNS_TOPPAR:ion.top
REMARK topology file 5  : CNS_TOPPAR:tpo.top
REMARK parameter file 1  : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2  : CNS_TOPPAR:dna-rna_rep.param
REMARK parameter file 3  : CNS_TOPPAR:water_rep.param
REMARK parameter file 4  : CNS_TOPPAR:ion.param
REMARK parameter file 5  : CNS_TOPPAR:tpo.param
REMARK molecular structure file: automatic
REMARK input coordinates: 36mod1.pdb
REMARK reflection file= remote.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 2.8
REMARK initial B-factor correction applied to fobs :
REMARK   B11=   1.580 B22=   1.580 B33=  -3.160
REMARK   B12=  -3.767 B13=   0.000 B23=   0.000
REMARK B-factor correction applied to coordinate array B:    0.915
REMARK bulk solvent: density level= 0.324998 e/A^3, B-factor= 34.4718 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK anomalous diffraction data was input
REMARK theoretical total number of refl. in resol. range: 107240 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0): 3377 (  3.1 % )
REMARK number of reflections rejected:                          0 (  0.0 % )
REMARK total number of reflections used:                   103863 ( 96.9 % )
REMARK number of reflections in working set:                93784 ( 87.5 % )
REMARK number of reflections in test set:                   10079 (  9.4 % )
CRYST1  107.669  107.669  168.300  90.00  90.00 120.00 P 32
```

```
REMARK FILENAME="ref37.pdb"
REMARK DATE:28-Jun-2002  13:23:24       created by user: orlicky
REMARK VERSION:1.1
ATOM      1  CB  SER A   2      72.279  75.039  74.638  1.00 40.45      A
ATOM      2  OG  SER A   2      72.875  75.230  73.368  1.00 36.62      A
ATOM      3  C   SER A   2      70.142  75.473  73.446  1.00 40.01      A
ATOM      4  O   SER A   2      69.547  74.397  73.338  1.00 39.92      A
ATOM      5  N   SER A   2      70.277  75.520  76.026  1.00 40.09      A
ATOM      6  CA  SER A   2      70.953  75.797  74.713  1.00 40.80      A
ATOM      7  N   ASN A   3      70.145  76.398  72.482  1.00 38.91      A
ATOM      8  CA  ASN A   3      69.428  76.196  71.221  1.00 37.67      A
ATOM      9  CB  ASN A   3      68.480  77.367  70.926  1.00 38.01      A
ATOM     10  CG  ASN A   3      67.193  77.305  71.736  1.00 38.13      A
ATOM     11  OD1 ASN A   3      66.616  76.236  71.944  1.00 38.39      A
ATOM     12  ND2 ASN A   3      66.733  78.458  72.184  1.00 36.20      A
ATOM     13  C   ASN A   3      70.310  75.996  69.990  1.00 35.89      A
ATOM     14  O   ASN A   3      71.503  76.275  69.995  1.00 34.48      A
ATOM     15  N   VAL A   4      69.685  75.500  68.928  1.00 36.46      A
ATOM     16  CA  VAL A   4      70.343  75.275  67.639  1.00 33.96      A
ATOM     17  CB  VAL A   4      70.545  73.750  67.383  1.00 33.36      A
ATOM     18  CG1 VAL A   4      70.533  73.449  65.916  1.00 33.70      A
ATOM     19  CG2 VAL A   4      71.855  73.295  67.985  1.00 34.50      A
ATOM     20  C   VAL A   4      69.415  75.889  66.584  1.00 31.88      A
ATOM     21  O   VAL A   4      68.209  76.036  66.818  1.00 31.04      A
ATOM     22  N   VAL A   5      69.972  76.282  65.443  1.00 31.25      A
ATOM     23  CA  VAL A   5      69.146  76.853  64.376  1.00 31.10      A
ATOM     24  CB  VAL A   5      69.458  78.346  64.086  1.00 31.85      A
ATOM     25  CG1 VAL A   5      68.586  78.825  62.927  1.00 32.81      A
ATOM     26  CG2 VAL A   5      69.188  79.192  65.314  1.00 31.47      A
ATOM     27  C   VAL A   5      69.339  76.075  63.089  1.00 29.35      A
ATOM     28  O   VAL A   5      70.448  75.952  62.588  1.00 29.57      A
ATOM     29  N   LEU A   6      68.232  75.561  62.574  1.00 28.63      A
ATOM     30  CA  LEU A   6      68.206  74.777  61.355  1.00 28.72      A
ATOM     31  CB  LEU A   6      67.299  73.558  61.559  1.00 27.60      A
ATOM     32  CG  LEU A   6      67.585  72.619  62.739  1.00 25.63      A
ATOM     33  CD1 LEU A   6      66.684  71.402  62.592  1.00 24.10      A
ATOM     34  CD2 LEU A   6      69.043  72.205  62.781  1.00 21.89      A
ATOM     35  C   LEU A   6      67.667  75.632  60.208  1.00 28.54      A
ATOM     36  O   LEU A   6      66.577  76.200  60.316  1.00 28.48      A
ATOM     37  N   VAL A   7      68.416  75.740  59.112  1.00 27.74      A
ATOM     38  CA  VAL A   7      67.945  76.548  57.978  1.00 25.90      A
ATOM     39  CB  VAL A   7      69.092  77.413  57.366  1.00 25.69      A
ATOM     40  CG1 VAL A   7      68.515  78.450  56.403  1.00 25.12      A
ATOM     41  CG2 VAL A   7      69.889  78.077  58.450  1.00 22.70      A
ATOM     42  C   VAL A   7      67.374  75.650  56.869  1.00 24.30      A
ATOM     43  O   VAL A   7      68.069  74.768  56.337  1.00 21.91      A
ATOM     44  N   SER A   8      66.111  75.881  56.522  1.00 23.21      A
ATOM     45  CA  SER A   8      65.453  75.091  55.486  1.00 23.15      A
ATOM     46  CB  SER A   8      63.966  75.433  55.375  1.00 21.22      A
ATOM     47  OG  SER A   8      63.794  76.735  54.826  1.00 20.44      A
ATOM     48  C   SER A   8      66.093  75.428  54.167  1.00 25.17      A
ATOM     49  O   SER A   8      66.851  76.389  54.054  1.00 27.53      A
ATOM     50  N   GLY A   9      65.782  74.635  53.155  1.00 26.78      A
ATOM     51  CA  GLY A   9      66.329  74.914  51.847  1.00 26.99      A
```

ATOM	52	C	GLY	A	9	65.726	76.208	51.320	1.00	27.95	A
ATOM	53	O	GLY	A	9	66.120	76.682	50.256	1.00	29.65	A
ATOM	54	N	GLU	A	10	64.762	76.782	52.039	1.00	26.66	A
ATOM	55	CA	GLU	A	10	64.160	78.025	51.582	1.00	25.22	A
ATOM	56	CB	GLU	A	10	62.637	77.927	51.610	1.00	24.78	A
ATOM	57	CG	GLU	A	10	62.045	76.721	50.905	1.00	24.26	A
ATOM	58	CD	GLU	A	10	60.543	76.567	51.203	1.00	27.17	A
ATOM	59	OE1	GLU	A	10	59.747	77.407	50.727	1.00	27.67	A
ATOM	60	OE2	GLU	A	10	60.144	75.617	51.929	1.00	28.38	A
ATOM	61	C	GLU	A	10	64.598	79.236	52.416	1.00	25.50	A
ATOM	62	O	GLU	A	10	63.853	80.213	52.538	1.00	24.72	A
ATOM	63	N	GLY	A	11	65.794	79.164	52.995	1.00	25.06	A
ATOM	64	CA	GLY	A	11	66.299	80.264	53.792	1.00	25.04	A
ATOM	65	C	GLY	A	11	65.740	80.473	55.192	1.00	25.64	A
ATOM	66	O	GLY	A	11	66.399	81.110	56.016	1.00	25.60	A
ATOM	67	N	GLU	A	12	64.552	79.946	55.483	1.00	26.56	A
ATOM	68	CA	GLU	A	12	63.945	80.113	56.806	1.00	27.47	A
ATOM	69	CB	GLU	A	12	62.510	79.614	56.782	1.00	26.92	A
ATOM	70	CG	GLU	A	12	61.661	80.451	55.874	1.00	32.01	A
ATOM	71	CD	GLU	A	12	60.215	80.003	55.841	1.00	35.92	A
ATOM	72	OE1	GLU	A	12	59.912	78.942	55.244	1.00	37.74	A
ATOM	73	OE2	GLU	A	12	59.367	80.716	56.419	1.00	39.01	A
ATOM	74	C	GLU	A	12	64.705	79.459	57.951	1.00	28.74	A
ATOM	75	O	GLU	A	12	65.222	78.345	57.826	1.00	29.61	A
ATOM	76	N	ARG	A	13	64.804	80.170	59.069	1.00	29.55	A
ATOM	77	CA	ARG	A	13	65.513	79.615	60.207	1.00	30.68	A
ATOM	78	CB	ARG	A	13	66.457	80.651	60.832	1.00	32.30	A
ATOM	79	CG	ARG	A	13	66.654	81.907	60.002	1.00	34.52	A
ATOM	80	CD	ARG	A	13	67.459	82.959	60.756	1.00	35.08	A
ATOM	81	NE	ARG	A	13	68.816	82.514	61.051	1.00	36.91	A
ATOM	82	CZ	ARG	A	13	69.454	82.778	62.188	1.00	37.09	A
ATOM	83	NH1	ARG	A	13	68.846	83.485	63.129	1.00	35.87	A
ATOM	84	NH2	ARG	A	13	70.691	82.328	62.391	1.00	37.00	A
ATOM	85	C	ARG	A	13	64.511	79.130	61.238	1.00	29.61	A
ATOM	86	O	ARG	A	13	63.494	79.783	61.506	1.00	29.30	A
ATOM	87	N	PHE	A	14	64.809	77.962	61.789	1.00	28.74	A
ATOM	88	CA	PHE	A	14	63.980	77.337	62.797	1.00	28.90	A
ATOM	89	CB	PHE	A	14	63.507	75.945	62.356	1.00	27.81	A
ATOM	90	CG	PHE	A	14	62.614	75.946	61.147	1.00	26.25	A
ATOM	91	CD1	PHE	A	14	63.149	75.925	59.867	1.00	25.67	A
ATOM	92	CD2	PHE	A	14	61.235	75.955	61.291	1.00	27.94	A
ATOM	93	CE1	PHE	A	14	62.324	75.912	58.745	1.00	25.90	A
ATOM	94	CE2	PHE	A	14	60.393	75.942	60.174	1.00	27.89	A
ATOM	95	CZ	PHE	A	14	60.940	75.921	58.896	1.00	26.23	A
ATOM	96	C	PHE	A	14	64.847	77.185	64.032	1.00	30.32	A
ATOM	97	O	PHE	A	14	66.004	76.760	63.959	1.00	30.71	A
ATOM	98	N	THR	A	15	64.305	77.558	65.176	1.00	32.94	A
ATOM	99	CA	THR	A	15	65.067	77.412	66.396	1.00	34.55	A
ATOM	100	CB	THR	A	15	64.910	78.650	67.275	1.00	34.81	A
ATOM	101	OG1	THR	A	15	65.362	79.797	66.548	1.00	35.82	A
ATOM	102	CG2	THR	A	15	65.737	78.509	68.541	1.00	36.02	A
ATOM	103	C	THR	A	15	64.535	76.179	67.119	1.00	34.29	A
ATOM	104	O	THR	A	15	63.358	75.830	66.984	1.00	35.01	A
ATOM	105	N	VAL	A	16	65.398	75.501	67.859	1.00	34.16	A

ATOM	106	CA	VAL	A	16	64.954	74.330	68.592	1.00	36.47	A
ATOM	107	CB	VAL	A	16	64.597	73.166	67.628	1.00	38.19	A
ATOM	108	CG1	VAL	A	16	65.697	72.981	66.579	1.00	37.94	A
ATOM	109	CG2	VAL	A	16	64.403	71.884	68.421	1.00	40.71	A
ATOM	110	C	VAL	A	16	65.992	73.862	69.601	1.00	36.55	A
ATOM	111	O	VAL	A	16	67.199	74.020	69.398	1.00	36.18	A
ATOM	112	N	ASP	A	17	65.511	73.294	70.699	1.00	36.09	A
ATOM	113	CA	ASP	A	17	66.398	72.817	71.750	1.00	36.61	A
ATOM	114	CB	ASP	A	17	65.586	72.082	72.812	1.00	38.44	A
ATOM	115	CG	ASP	A	17	66.458	71.416	73.840	1.00	40.95	A
ATOM	116	OD1	ASP	A	17	66.418	70.164	73.924	1.00	43.10	A
ATOM	117	OD2	ASP	A	17	67.184	72.137	74.556	1.00	41.69	A
ATOM	118	C	ASP	A	17	67.499	71.902	71.196	1.00	35.77	A
ATOM	119	O	ASP	A	17	67.218	70.903	70.543	1.00	33.05	A
ATOM	120	N	LYS	A	18	68.757	72.245	71.471	1.00	36.17	A
ATOM	121	CA	LYS	A	18	69.897	71.473	70.972	1.00	35.91	A
ATOM	122	CB	LYS	A	18	71.208	72.003	71.541	1.00	35.90	A
ATOM	123	CG	LYS	A	18	72.397	71.086	71.239	1.00	36.70	A
ATOM	124	CD	LYS	A	18	73.679	71.525	71.964	1.00	37.63	A
ATOM	125	CE	LYS	A	18	74.131	72.918	71.523	1.00	38.26	A
ATOM	126	NZ	LYS	A	18	75.528	73.223	71.956	1.00	38.28	A
ATOM	127	C	LYS	A	18	69.776	70.010	71.319	1.00	36.47	A
ATOM	128	O	LYS	A	18	70.048	69.129	70.497	1.00	35.04	A
ATOM	129	N	LYS	A	19	69.388	69.756	72.559	1.00	38.15	A
ATOM	130	CA	LYS	A	19	69.220	68.393	73.011	1.00	38.79	A
ATOM	131	CB	LYS	A	19	68.733	68.374	74.456	1.00	39.52	A
ATOM	132	CG	LYS	A	19	68.597	66.980	75.018	0.00	40.07	A
ATOM	133	CD	LYS	A	19	68.074	66.996	76.439	0.00	40.81	A
ATOM	134	CE	LYS	A	19	66.638	67.489	76.505	0.00	41.30	A
ATOM	135	NZ	LYS	A	19	66.086	67.373	77.885	0.00	41.65	A
ATOM	136	C	LYS	A	19	68.202	67.734	72.084	1.00	38.59	A
ATOM	137	O	LYS	A	19	68.508	66.734	71.445	1.00	39.10	A
ATOM	138	N	ILE	A	20	67.004	68.304	71.984	1.00	37.46	A
ATOM	139	CA	ILE	A	20	65.991	67.725	71.112	1.00	37.39	A
ATOM	140	CB	ILE	A	20	64.685	68.503	71.168	1.00	36.72	A
ATOM	141	CG2	ILE	A	20	63.687	67.918	70.167	1.00	36.45	A
ATOM	142	CG1	ILE	A	20	64.118	68.440	72.572	1.00	35.02	A
ATOM	143	CD1	ILE	A	20	62.910	69.280	72.751	1.00	36.54	A
ATOM	144	C	ILE	A	20	66.432	67.678	69.660	1.00	37.89	A
ATOM	145	O	ILE	A	20	66.157	66.718	68.954	1.00	38.16	A
ATOM	146	N	ALA	A	21	67.125	68.717	69.218	1.00	39.24	A
ATOM	147	CA	ALA	A	21	67.591	68.793	67.843	1.00	38.28	A
ATOM	148	CB	ALA	A	21	68.197	70.154	67.570	1.00	38.24	A
ATOM	149	C	ALA	A	21	68.609	67.719	67.589	1.00	38.38	A
ATOM	150	O	ALA	A	21	68.798	67.294	66.455	1.00	38.91	A
ATOM	151	N	GLU	A	22	69.281	67.276	68.640	1.00	38.98	A
ATOM	152	CA	GLU	A	22	70.280	66.242	68.449	1.00	39.28	A
ATOM	153	CB	GLU	A	22	71.102	66.063	69.717	1.00	42.76	A
ATOM	154	CG	GLU	A	22	72.116	67.162	69.962	1.00	47.53	A
ATOM	155	CD	GLU	A	22	72.856	66.948	71.259	1.00	50.36	A
ATOM	156	OE1	GLU	A	22	73.381	65.827	71.444	1.00	50.70	A
ATOM	157	OE2	GLU	A	22	72.907	67.891	72.089	1.00	52.73	A
ATOM	158	C	GLU	A	22	69.666	64.913	68.021	1.00	37.58	A
ATOM	159	O	GLU	A	22	70.391	63.955	67.805	1.00	37.40	A

ATOM	160	N	ARG	A	23	68.342	64.850	67.890	1.00	36.03	A
ATOM	161	CA	ARG	A	23	67.706	63.615	67.459	1.00	34.62	A
ATOM	162	CB	ARG	A	23	66.200	63.765	67.306	1.00	33.59	A
ATOM	163	CG	ARG	A	23	65.509	62.431	67.022	1.00	33.69	A
ATOM	164	CD	ARG	A	23	65.708	61.463	68.191	1.00	33.70	A
ATOM	165	NE	ARG	A	23	64.457	61.196	68.901	1.00	34.45	A
ATOM	166	CZ	ARG	A	23	64.360	60.622	70.100	1.00	33.77	A
ATOM	167	NH1	ARG	A	23	65.447	60.243	70.764	1.00	34.73	A
ATOM	168	NH2	ARG	A	23	63.164	60.414	70.633	1.00	29.73	A
ATOM	169	C	ARG	A	23	68.270	63.248	66.116	1.00	35.80	A
ATOM	170	O	ARG	A	23	68.362	62.077	65.769	1.00	37.71	A
ATOM	171	N	SER	A	24	68.629	64.266	65.345	1.00	37.45	A
ATOM	172	CA	SER	A	24	69.208	64.072	64.018	1.00	37.69	A
ATOM	173	CB	SER	A	24	69.047	65.344	63.187	1.00	36.12	A
ATOM	174	OG	SER	A	24	69.929	65.337	62.084	1.00	32.96	A
ATOM	175	C	SER	A	24	70.686	63.729	64.127	1.00	38.12	A
ATOM	176	O	SER	A	24	71.506	64.581	64.466	1.00	36.69	A
ATOM	177	N	LEU	A	25	71.022	62.478	63.837	1.00	40.01	A
ATOM	178	CA	LEU	A	25	72.409	62.036	63.901	1.00	42.65	A
ATOM	179	CB	LEU	A	25	72.534	60.580	63.436	1.00	43.67	A
ATOM	180	CG	LEU	A	25	71.996	59.493	64.383	1.00	43.11	A
ATOM	181	CD1	LEU	A	25	72.208	58.104	63.794	1.00	41.75	A
ATOM	182	CD2	LEU	A	25	72.703	59.615	65.713	1.00	41.72	A
ATOM	183	C	LEU	A	25	73.313	62.916	63.054	1.00	42.76	A
ATOM	184	O	LEU	A	25	74.475	63.112	63.394	1.00	42.58	A
ATOM	185	N	LEU	A	26	72.779	63.442	61.954	1.00	44.29	A
ATOM	186	CA	LEU	A	26	73.554	64.309	61.070	1.00	46.11	A
ATOM	187	CB	LEU	A	26	72.701	64.742	59.875	1.00	46.16	A
ATOM	188	CG	LEU	A	26	73.318	65.721	58.868	1.00	45.56	A
ATOM	189	CD1	LEU	A	26	74.571	65.123	58.268	1.00	44.90	A
ATOM	190	CD2	LEU	A	26	72.303	66.050	57.774	1.00	45.90	A
ATOM	191	C	LEU	A	26	73.992	65.524	61.866	1.00	47.66	A
ATOM	192	O	LEU	A	26	75.140	65.962	61.770	1.00	47.34	A
ATOM	193	N	LEU	A	27	73.060	66.055	62.655	1.00	50.27	A
ATOM	194	CA	LEU	A	27	73.312	67.212	63.508	1.00	52.62	A
ATOM	195	CB	LEU	A	27	71.985	67.831	63.963	1.00	52.60	A
ATOM	196	CG	LEU	A	27	72.112	68.911	65.046	1.00	52.80	A
ATOM	197	CD1	LEU	A	27	72.872	70.114	64.501	1.00	52.04	A
ATOM	198	CD2	LEU	A	27	70.729	69.314	65.513	1.00	52.96	A
ATOM	199	C	LEU	A	27	74.145	66.835	64.742	1.00	54.44	A
ATOM	200	O	LEU	A	27	75.085	67.540	65.100	1.00	54.34	A
ATOM	201	N	LYS	A	28	73.786	65.726	65.387	1.00	56.05	A
ATOM	202	CA	LYS	A	28	74.491	65.255	66.574	1.00	57.53	A
ATOM	203	CB	LYS	A	28	73.880	63.942	67.059	1.00	58.27	A
ATOM	204	CG	LYS	A	28	74.486	63.418	68.347	0.00	58.77	A
ATOM	205	CD	LYS	A	28	73.864	62.093	68.750	0.00	59.35	A
ATOM	206	CE	LYS	A	28	74.520	61.545	70.004	0.00	59.70	A
ATOM	207	NZ	LYS	A	28	73.986	60.205	70.367	0.00	59.95	A
ATOM	208	C	LYS	A	28	75.974	65.049	66.297	0.00	58.99	A
ATOM	209	O	LYS	A	28	76.811	65.183	67.191	0.00	58.95	A
ATOM	210	N	ASN	A	29	76.290	64.716	65.052	1.00	60.36	A
ATOM	211	CA	ASN	A	29	77.667	64.489	64.647	1.00	62.38	A
ATOM	212	CB	ASN	A	29	77.729	63.509	63.484	1.00	63.15	A
ATOM	213	CG	ASN	A	29	77.458	62.085	63.908	1.00	64.88	A

```
ATOM    214  OD1 ASN A  29      77.410  61.185  63.068  1.00 67.16      A
ATOM    215  ND2 ASN A  29      77.285  61.865  65.215  1.00 64.20      A
ATOM    216  C   ASN A  29      78.326  65.778  64.227  1.00 63.19      A
ATOM    217  O   ASN A  29      79.547  65.852  64.106  1.00 63.26      A
ATOM    218  N   TYR A  30      77.514  66.797  63.993  1.00 64.46      A
ATOM    219  CA  TYR A  30      78.049  68.083  63.583  1.00 65.53      A
ATOM    220  CB  TYR A  30      76.898  69.085  63.417  1.00 67.82      A
ATOM    221  CG  TYR A  30      77.127  70.172  62.379  1.00 68.70      A
ATOM    222  CD1 TYR A  30      77.416  69.853  61.050  1.00 68.47      A
ATOM    223  CE1 TYR A  30      77.595  70.854  60.092  1.00 69.31      A
ATOM    224  CD2 TYR A  30      77.024  71.522  62.722  1.00 68.53      A
ATOM    225  CE2 TYR A  30      77.201  72.528  61.774  1.00 69.17      A
ATOM    226  CZ  TYR A  30      77.485  72.190  60.464  1.00 69.54      A
ATOM    227  OH  TYR A  30      77.651  73.191  59.534  1.00 69.67      A
ATOM    228  C   TYR A  30      79.043  68.550  64.658  1.00 65.21      A
ATOM    229  O   TYR A  30      79.894  69.395  64.391  1.00 64.91      A
ATOM    230  N   VAL A  31      78.935  67.964  65.856  1.00 64.85      A
ATOM    231  CA  VAL A  31      79.786  68.271  67.019  1.00 62.98      A
ATOM    232  CB  VAL A  31      81.049  67.351  67.096  1.00 62.18      A
ATOM    233  CG1 VAL A  31      80.624  65.903  67.216  1.00 61.36      A
ATOM    234  CG2 VAL A  31      81.961  67.562  65.882  1.00 60.58      A
ATOM    235  C   VAL A  31      80.256  69.712  67.123  1.00 62.08      A
ATOM    236  O   VAL A  31      80.624  70.168  68.203  1.00 60.74      A
ATOM    237  N   ILE A  45      76.524  76.394  65.711  1.00 42.05      A
ATOM    238  CA  ILE A  45      75.216  76.668  66.290  1.00 41.90      A
ATOM    239  CB  ILE A  45      75.276  77.864  67.310  1.00 42.05      A
ATOM    240  CG2 ILE A  45      75.089  79.191  66.601  1.00 40.06      A
ATOM    241  CG1 ILE A  45      74.171  77.726  68.363  1.00 43.22      A
ATOM    242  CD1 ILE A  45      74.407  76.620  69.388  1.00 43.84      A
ATOM    243  C   ILE A  45      74.180  76.963  65.195  1.00 41.36      A
ATOM    244  O   ILE A  45      73.021  77.252  65.488  1.00 41.48      A
ATOM    245  N   VAL A  46      74.592  76.918  63.933  1.00 39.64      A
ATOM    246  CA  VAL A  46      73.635  77.132  62.849  1.00 39.19      A
ATOM    247  CB  VAL A  46      73.675  78.579  62.293  1.00 37.60      A
ATOM    248  CG1 VAL A  46      72.665  78.729  61.166  1.00 35.40      A
ATOM    249  CG2 VAL A  46      73.346  79.567  63.390  1.00 38.18      A
ATOM    250  C   VAL A  46      73.917  76.159  61.715  1.00 39.41      A
ATOM    251  O   VAL A  46      74.815  76.385  60.905  1.00 41.28      A
ATOM    252  N   MSE A  47      73.160  75.069  61.655  1.00 38.13      A
ATOM    253  CA  MSE A  47      73.390  74.093  60.606  1.00 37.60      A
ATOM    254  CB  MSE A  47      73.419  72.680  61.169  1.00 40.79      A
ATOM    255  CG  MSE A  47      73.777  71.642  60.118  1.00 44.02      A
ATOM    256  SE  MSE A  47      73.314  69.875  60.679  1.00 50.37      A
ATOM    257  CE  MSE A  47      71.388  70.111  60.653  1.00 48.04      A
ATOM    258  C   MSE A  47      72.402  74.138  59.465  1.00 36.07      A
ATOM    259  O   MSE A  47      71.195  74.213  59.670  1.00 36.45      A
ATOM    260  N   PRO A  48      72.917  74.093  58.229  1.00 34.97      A
ATOM    261  CD  PRO A  48      74.305  74.434  57.870  1.00 34.19      A
ATOM    262  CA  PRO A  48      72.066  74.128  57.040  1.00 34.14      A
ATOM    263  CB  PRO A  48      73.041  74.516  55.929  1.00 33.07      A
ATOM    264  CG  PRO A  48      74.103  75.290  56.654  1.00 33.93      A
ATOM    265  C   PRO A  48      71.369  72.806  56.729  1.00 33.52      A
ATOM    266  O   PRO A  48      71.922  71.727  56.946  1.00 32.95      A
ATOM    267  N   VAL A  49      70.140  72.906  56.231  1.00 32.78      A
```

```
ATOM    268  CA  VAL A  49      69.383  71.731  55.828  1.00 32.43      A
ATOM    269  CB  VAL A  49      68.073  71.538  56.671  1.00 31.33      A
ATOM    270  CG1 VAL A  49      67.575  70.120  56.539  1.00 30.50      A
ATOM    271  CG2 VAL A  49      68.327  71.845  58.141  1.00 34.13      A
ATOM    272  C   VAL A  49      69.062  71.991  54.340  1.00 32.95      A
ATOM    273  O   VAL A  49      67.958  72.412  53.977  1.00 32.24      A
ATOM    274  N   PRO A  50      70.060  71.757  53.460  1.00 33.40      A
ATOM    275  CD  PRO A  50      71.393  71.237  53.811  1.00 33.34      A
ATOM    276  CA  PRO A  50      69.971  71.942  52.010  1.00 32.39      A
ATOM    277  CB  PRO A  50      71.310  71.409  51.512  1.00 32.52      A
ATOM    278  CG  PRO A  50      72.217  71.682  52.627  1.00 33.15      A
ATOM    279  C   PRO A  50      68.813  71.229  51.343  1.00 31.05      A
ATOM    280  O   PRO A  50      68.509  70.079  51.648  1.00 31.50      A
ATOM    281  N   ASN A  51      68.176  71.936  50.420  1.00 30.37      A
ATOM    282  CA  ASN A  51      67.071  71.387  49.645  1.00 30.66      A
ATOM    283  CB  ASN A  51      67.648  70.432  48.595  1.00 31.76      A
ATOM    284  CG  ASN A  51      69.069  70.813  48.175  1.00 30.85      A
ATOM    285  OD1 ASN A  51      69.262  71.794  47.478  1.00 27.98      A
ATOM    286  ND2 ASN A  51      70.072  70.031  48.620  1.00 33.14      A
ATOM    287  C   ASN A  51      65.978  70.665  50.450  1.00 29.20      A
ATOM    288  O   ASN A  51      65.588  69.551  50.120  1.00 26.62      A
ATOM    289  N   VAL A  52      65.500  71.292  51.512  1.00 29.33      A
ATOM    290  CA  VAL A  52      64.435  70.692  52.283  1.00 29.38      A
ATOM    291  CB  VAL A  52      64.913  70.157  53.640  1.00 30.20      A
ATOM    292  CG1 VAL A  52      63.747  69.506  54.390  1.00 26.29      A
ATOM    293  CG2 VAL A  52      66.022  69.129  53.420  1.00 29.10      A
ATOM    294  C   VAL A  52      63.401  71.774  52.492  1.00 29.83      A
ATOM    295  O   VAL A  52      63.693  72.821  53.058  1.00 29.62      A
ATOM    296  N   ARG A  53      62.199  71.504  51.992  1.00 30.70      A
ATOM    297  CA  ARG A  53      61.064  72.411  52.063  1.00 31.16      A
ATOM    298  CB  ARG A  53      59.814  71.667  51.580  1.00 35.30      A
ATOM    299  CG  ARG A  53      58.775  72.499  50.846  1.00 39.79      A
ATOM    300  CD  ARG A  53      57.564  71.636  50.474  1.00 42.92      A
ATOM    301  NE  ARG A  53      56.700  72.283  49.491  1.00 47.91      A
ATOM    302  CZ  ARG A  53      55.889  73.308  49.749  1.00 50.95      A
ATOM    303  NH1 ARG A  53      55.815  73.814  50.972  1.00 53.87      A
ATOM    304  NH2 ARG A  53      55.158  73.844  48.776  1.00 52.85      A
ATOM    305  C   ARG A  53      60.864  72.876  53.505  1.00 30.38      A
ATOM    306  O   ARG A  53      60.860  72.068  54.425  1.00 31.84      A
ATOM    307  N   SER A  54      60.694  74.173  53.708  1.00 27.65      A
ATOM    308  CA  SER A  54      60.481  74.670  55.050  1.00 24.25      A
ATOM    309  CB  SER A  54      60.094  76.142  55.013  1.00 23.48      A
ATOM    310  OG  SER A  54      61.197  76.935  54.642  1.00 22.07      A
ATOM    311  C   SER A  54      59.386  73.866  55.742  1.00 22.74      A
ATOM    312  O   SER A  54      59.611  73.280  56.792  1.00 21.74      A
ATOM    313  N   SER A  55      58.204  73.835  55.143  1.00 22.72      A
ATOM    314  CA  SER A  55      57.078  73.114  55.707  1.00 22.82      A
ATOM    315  CB  SER A  55      55.913  73.117  54.736  1.00 20.88      A
ATOM    316  OG  SER A  55      56.159  72.211  53.683  1.00 23.15      A
ATOM    317  C   SER A  55      57.432  71.670  56.042  1.00 24.40      A
ATOM    318  O   SER A  55      56.780  71.034  56.877  1.00 27.21      A
ATOM    319  N   VAL A  56      58.457  71.144  55.387  1.00 21.45      A
ATOM    320  CA  VAL A  56      58.862  69.782  55.662  1.00 20.79      A
ATOM    321  CB  VAL A  56      59.648  69.194  54.488  1.00 19.14      A
```

```
ATOM    322  CG1 VAL A  56      60.254  67.875  54.889  1.00 16.99      A
ATOM    323  CG2 VAL A  56      58.738  69.029  53.301  1.00 18.04      A
ATOM    324  C   VAL A  56      59.719  69.727  56.924  1.00 21.47      A
ATOM    325  O   VAL A  56      59.498  68.903  57.797  1.00 21.73      A
ATOM    326  N   LEU A  57      60.703  70.606  57.010  1.00 22.90      A
ATOM    327  CA  LEU A  57      61.573  70.645  58.159  1.00 24.53      A
ATOM    328  CB  LEU A  57      62.647  71.696  57.937  1.00 24.08      A
ATOM    329  CG  LEU A  57      63.681  71.859  59.042  1.00 24.59      A
ATOM    330  CD1 LEU A  57      64.030  70.523  59.664  1.00 23.09      A
ATOM    331  CD2 LEU A  57      64.924  72.530  58.438  1.00 23.83      A
ATOM    332  C   LEU A  57      60.760  70.949  59.411  1.00 27.00      A
ATOM    333  O   LEU A  57      61.044  70.424  60.486  1.00 27.31      A
ATOM    334  N   GLN A  58      59.740  71.790  59.270  1.00 28.60      A
ATOM    335  CA  GLN A  58      58.885  72.133  60.402  1.00 29.92      A
ATOM    336  CB  GLN A  58      57.789  73.112  59.979  1.00 29.50      A
ATOM    337  CG  GLN A  58      56.729  73.358  61.044  1.00 29.08      A
ATOM    338  CD  GLN A  58      55.975  74.654  60.815  1.00 27.90      A
ATOM    339  OE1 GLN A  58      56.591  75.700  60.657  1.00 30.17      A
ATOM    340  NE2 GLN A  58      54.648  74.594  60.802  1.00 25.55      A
ATOM    341  C   GLN A  58      58.257  70.845  60.886  1.00 30.93      A
ATOM    342  O   GLN A  58      58.354  70.483  62.065  1.00 33.35      A
ATOM    343  N   LYS A  59      57.609  70.156  59.955  1.00 30.29      A
ATOM    344  CA  LYS A  59      56.976  68.880  60.248  1.00 29.48      A
ATOM    345  CB  LYS A  59      56.581  68.209  58.937  1.00 28.21      A
ATOM    346  CG  LYS A  59      55.283  67.470  58.978  1.00 29.03      A
ATOM    347  CD  LYS A  59      54.108  68.397  59.081  1.00 27.32      A
ATOM    348  CE  LYS A  59      52.834  67.608  58.857  1.00 26.80      A
ATOM    349  NZ  LYS A  59      52.804  66.508  59.824  1.00 25.00      A
ATOM    350  C   LYS A  59      58.004  68.017  61.006  1.00 29.46      A
ATOM    351  O   LYS A  59      57.709  67.465  62.070  1.00 29.02      A
ATOM    352  N   VAL A  60      59.217  67.929  60.467  1.00 28.15      A
ATOM    353  CA  VAL A  60      60.259  67.142  61.106  1.00 28.14      A
ATOM    354  CB  VAL A  60      61.573  67.226  60.319  1.00 28.15      A
ATOM    355  CG1 VAL A  60      62.731  66.715  61.152  1.00 27.46      A
ATOM    356  CG2 VAL A  60      61.455  66.386  59.060  1.00 29.05      A
ATOM    357  C   VAL A  60      60.495  67.574  62.543  1.00 28.57      A
ATOM    358  O   VAL A  60      60.434  66.762  63.465  1.00 29.28      A
ATOM    359  N   ILE A  61      60.768  68.853  62.734  1.00 28.79      A
ATOM    360  CA  ILE A  61      61.007  69.375  64.068  1.00 28.54      A
ATOM    361  CB  ILE A  61      61.195  70.903  64.001  1.00 27.31      A
ATOM    362  CG2 ILE A  61      61.238  71.501  65.391  1.00 26.36      A
ATOM    363  CG1 ILE A  61      62.482  71.202  63.223  1.00 27.68      A
ATOM    364  CD1 ILE A  61      62.737  72.660  62.979  1.00 27.54      A
ATOM    365  C   ILE A  61      59.860  69.020  65.016  1.00 29.35      A
ATOM    366  O   ILE A  61      60.086  68.538  66.131  1.00 27.58      A
ATOM    367  N   GLU A  62      58.627  69.247  64.572  1.00 30.00      A
ATOM    368  CA  GLU A  62      57.473  68.949  65.415  1.00 31.73      A
ATOM    369  CB  GLU A  62      56.169  69.203  64.667  1.00 29.92      A
ATOM    370  CG  GLU A  62      55.043  68.328  65.181  1.00 30.57      A
ATOM    371  CD  GLU A  62      53.688  68.775  64.703  1.00 31.86      A
ATOM    372  OE1 GLU A  62      53.530  68.966  63.470  1.00 33.09      A
ATOM    373  OE2 GLU A  62      52.781  68.934  65.562  1.00 31.63      A
ATOM    374  C   GLU A  62      57.480  67.505  65.907  1.00 32.78      A
ATOM    375  O   GLU A  62      57.035  67.207  67.017  1.00 32.73      A
```

ATOM	376	N	TRP	A	63	57.965	66.610	65.057	1.00	34.15	A
ATOM	377	CA	TRP	A	63	58.029	65.204	65.394	1.00	34.37	A
ATOM	378	CB	TRP	A	63	58.259	64.380	64.127	1.00	33.74	A
ATOM	379	CG	TRP	A	63	58.189	62.915	64.354	1.00	31.94	A
ATOM	380	CD2	TRP	A	63	59.254	62.071	64.798	1.00	30.34	A
ATOM	381	CE2	TRP	A	63	58.729	60.775	64.937	1.00	29.79	A
ATOM	382	CE3	TRP	A	63	60.601	62.287	65.104	1.00	29.39	A
ATOM	383	CD1	TRP	A	63	57.092	62.120	64.235	1.00	31.15	A
ATOM	384	NE1	TRP	A	63	57.406	60.829	64.584	1.00	30.29	A
ATOM	385	CZ2	TRP	A	63	59.506	59.698	65.361	1.00	29.60	A
ATOM	386	CZ3	TRP	A	63	61.372	61.211	65.528	1.00	28.85	A
ATOM	387	CH2	TRP	A	63	60.821	59.937	65.654	1.00	27.95	A
ATOM	388	C	TRP	A	63	59.181	64.989	66.372	1.00	34.92	A
ATOM	389	O	TRP	A	63	59.146	64.078	67.182	1.00	36.00	A
ATOM	390	N	ALA	A	64	60.195	65.840	66.316	1.00	35.06	A
ATOM	391	CA	ALA	A	64	61.332	65.673	67.207	1.00	36.52	A
ATOM	392	CB	ALA	A	64	62.567	66.371	66.621	1.00	35.61	A
ATOM	393	C	ALA	A	64	61.071	66.166	68.636	1.00	38.06	A
ATOM	394	O	ALA	A	64	61.606	65.607	69.602	1.00	38.15	A
ATOM	395	N	GLU	A	65	60.266	67.218	68.764	1.00	38.68	A
ATOM	396	CA	GLU	A	65	59.934	67.776	70.063	1.00	38.24	A
ATOM	397	CB	GLU	A	65	59.405	69.201	69.912	1.00	38.18	A
ATOM	398	CG	GLU	A	65	60.459	70.151	69.397	1.00	38.80	A
ATOM	399	CD	GLU	A	65	59.895	71.454	68.840	1.00	39.78	A
ATOM	400	OE1	GLU	A	65	58.673	71.527	68.547	1.00	38.29	A
ATOM	401	OE2	GLU	A	65	60.695	72.408	68.683	1.00	39.80	A
ATOM	402	C	GLU	A	65	58.879	66.902	70.708	1.00	38.37	A
ATOM	403	O	GLU	A	65	58.835	66.742	71.925	1.00	39.26	A
ATOM	404	N	HIS	A	66	58.024	66.312	69.896	1.00	38.38	A
ATOM	405	CA	HIS	A	66	57.006	65.482	70.479	1.00	40.16	A
ATOM	406	CB	HIS	A	66	55.929	65.179	69.465	1.00	39.56	A
ATOM	407	CG	HIS	A	66	54.902	64.215	69.955	1.00	39.86	A
ATOM	408	CD2	HIS	A	66	53.613	64.399	70.320	1.00	39.39	A
ATOM	409	ND1	HIS	A	66	55.137	62.859	70.036	1.00	38.45	A
ATOM	410	CE1	HIS	A	66	54.031	62.248	70.418	1.00	38.21	A
ATOM	411	NE2	HIS	A	66	53.091	63.159	70.595	1.00	39.69	A
ATOM	412	C	HIS	A	66	57.616	64.205	71.002	1.00	42.15	A
ATOM	413	O	HIS	A	66	57.115	63.619	71.959	1.00	44.74	A
ATOM	414	N	HIS	A	67	58.701	63.775	70.377	1.00	43.11	A
ATOM	415	CA	HIS	A	67	59.388	62.573	70.807	1.00	44.64	A
ATOM	416	CB	HIS	A	67	59.711	61.681	69.598	1.00	43.57	A
ATOM	417	CG	HIS	A	67	58.524	60.951	69.046	1.00	42.88	A
ATOM	418	CD2	HIS	A	67	58.088	59.684	69.241	1.00	42.35	A
ATOM	419	ND1	HIS	A	67	57.615	61.540	68.194	1.00	43.39	A
ATOM	420	CE1	HIS	A	67	56.673	60.667	67.886	1.00	41.93	A
ATOM	421	NE2	HIS	A	67	56.936	59.533	68.508	1.00	40.92	A
ATOM	422	C	HIS	A	67	60.673	62.989	71.512	1.00	46.18	A
ATOM	423	O	HIS	A	67	61.767	62.552	71.144	1.00	47.55	A
ATOM	424	N	ARG	A	68	60.541	63.842	72.524	1.00	47.19	A
ATOM	425	CA	ARG	A	68	61.704	64.322	73.270	1.00	48.05	A
ATOM	426	CB	ARG	A	68	61.390	65.665	73.959	1.00	47.55	A
ATOM	427	CG	ARG	A	68	60.459	65.576	75.163	1.00	47.12	A
ATOM	428	CD	ARG	A	68	60.219	66.943	75.813	1.00	45.40	A
ATOM	429	NE	ARG	A	68	59.137	67.657	75.151	1.00	44.72	A

ATOM	430	CZ	ARG	A	68	57.849	67.387	75.342	1.00	44.29	A
ATOM	431	NH1	ARG	A	68	57.485	66.434	76.179	1.00	46.93	A
ATOM	432	NH2	ARG	A	68	56.915	68.043	74.678	1.00	45.61	A
ATOM	433	C	ARG	A	68	62.187	63.308	74.303	1.00	49.19	A
ATOM	434	O	ARG	A	68	63.383	63.228	74.593	1.00	48.48	A
ATOM	435	N	ASP	A	69	61.261	62.525	74.848	1.00	51.12	A
ATOM	436	CA	ASP	A	69	61.626	61.531	75.853	1.00	52.05	A
ATOM	437	CB	ASP	A	69	60.967	61.862	77.187	1.00	50.12	A
ATOM	438	CG	ASP	A	69	61.351	63.221	77.684	1.00	49.36	A
ATOM	439	OD1	ASP	A	69	62.572	63.496	77.736	1.00	48.50	A
ATOM	440	OD2	ASP	A	69	60.440	64.010	78.015	1.00	49.39	A
ATOM	441	C	ASP	A	69	61.245	60.126	75.442	1.00	52.86	A
ATOM	442	O	ASP	A	69	60.787	59.335	76.261	1.00	52.94	A
ATOM	443	N	SER	A	70	61.437	59.812	74.170	1.00	54.02	A
ATOM	444	CA	SER	A	70	61.106	58.488	73.690	1.00	55.97	A
ATOM	445	CB	SER	A	70	60.259	58.588	72.425	1.00	54.70	A
ATOM	446	OG	SER	A	70	59.031	59.239	72.703	1.00	54.60	A
ATOM	447	C	SER	A	70	62.379	57.702	73.425	1.00	58.22	A
ATOM	448	O	SER	A	70	63.463	58.273	73.306	1.00	58.71	A
ATOM	449	N	ASN	A	71	62.252	56.385	73.362	1.00	60.80	A
ATOM	450	CA	ASN	A	71	63.403	55.545	73.105	1.00	64.11	A
ATOM	451	CB	ASN	A	71	63.999	55.049	74.421	1.00	62.74	A
ATOM	452	CG	ASN	A	71	64.012	56.121	75.495	1.00	62.42	A
ATOM	453	OD1	ASN	A	71	63.016	56.332	76.183	1.00	61.70	A
ATOM	454	ND2	ASN	A	71	65.139	56.811	75.636	1.00	62.41	A
ATOM	455	C	ASN	A	71	62.957	54.377	72.247	1.00	67.50	A
ATOM	456	O	ASN	A	71	62.140	53.558	72.669	1.00	68.91	A
ATOM	457	N	PHE	A	72	63.486	54.313	71.030	1.00	70.54	A
ATOM	458	CA	PHE	A	72	63.134	53.245	70.110	1.00	72.15	A
ATOM	459	CB	PHE	A	72	62.792	53.827	68.721	1.00	72.15	A
ATOM	460	CG	PHE	A	72	61.940	55.087	68.759	1.00	71.12	A
ATOM	461	CD1	PHE	A	72	62.539	56.349	68.784	1.00	70.74	A
ATOM	462	CD2	PHE	A	72	60.546	55.012	68.765	1.00	70.32	A
ATOM	463	CE1	PHE	A	72	61.767	57.514	68.814	1.00	70.31	A
ATOM	464	CE2	PHE	A	72	59.768	56.173	68.796	1.00	70.64	A
ATOM	465	CZ	PHE	A	72	60.383	57.425	68.821	1.00	70.21	A
ATOM	466	C	PHE	A	72	64.307	52.261	70.001	1.00	73.60	A
ATOM	467	O	PHE	A	72	65.466	52.623	70.226	1.00	73.93	A
ATOM	468	N	PRO	A	73	64.012	50.992	69.685	1.00	75.25	A
ATOM	469	CD	PRO	A	73	62.656	50.410	69.635	1.00	75.90	A
ATOM	470	CA	PRO	A	73	65.039	49.952	69.545	1.00	75.83	A
ATOM	471	CB	PRO	A	73	64.230	48.732	69.122	1.00	76.63	A
ATOM	472	CG	PRO	A	73	62.924	48.937	69.852	1.00	76.34	A
ATOM	473	C	PRO	A	73	66.099	50.325	68.511	0.00	76.16	A
ATOM	474	O	PRO	A	73	67.292	50.365	68.813	0.00	76.37	A
ATOM	475	N	VAL	A	86	52.596	52.678	63.351	1.00	68.06	A
ATOM	476	CA	VAL	A	86	52.119	51.882	64.474	1.00	69.23	A
ATOM	477	CB	VAL	A	86	53.259	50.998	65.073	1.00	69.13	A
ATOM	478	CG1	VAL	A	86	52.716	50.130	66.203	1.00	68.76	A
ATOM	479	CG2	VAL	A	86	53.864	50.111	63.989	1.00	69.85	A
ATOM	480	C	VAL	A	86	51.576	52.809	65.562	1.00	69.62	A
ATOM	481	O	VAL	A	86	50.459	52.627	66.061	1.00	69.53	A
ATOM	482	N	ASP	A	87	52.368	53.821	65.907	1.00	69.73	A
ATOM	483	CA	ASP	A	87	51.995	54.792	66.936	1.00	68.97	A

ATOM	484	CB	ASP	A	87	53.177	55.726	67.223	1.00	70.05	A
ATOM	485	CG	ASP	A	87	52.982	56.555	68.487	1.00	70.55	A
ATOM	486	OD1	ASP	A	87	52.047	57.386	68.514	1.00	70.97	A
ATOM	487	OD2	ASP	A	87	53.768	56.374	69.447	1.00	69.47	A
ATOM	488	C	ASP	A	87	50.766	55.609	66.528	1.00	67.85	A
ATOM	489	O	ASP	A	87	50.574	55.925	65.353	1.00	67.51	A
ATOM	490	N	SER	A	88	49.936	55.948	67.510	1.00	66.47	A
ATOM	491	CA	SER	A	88	48.714	56.708	67.263	1.00	64.69	A
ATOM	492	CB	SER	A	88	47.872	56.772	68.537	1.00	65.29	A
ATOM	493	OG	SER	A	88	46.724	57.579	68.337	1.00	66.37	A
ATOM	494	C	SER	A	88	48.976	58.124	66.770	1.00	62.66	A
ATOM	495	O	SER	A	88	48.420	58.553	65.755	1.00	61.70	A
ATOM	496	N	TRP	A	89	49.824	58.843	67.498	1.00	60.57	A
ATOM	497	CA	TRP	A	89	50.161	60.221	67.160	1.00	58.68	A
ATOM	498	CB	TRP	A	89	50.999	60.836	68.281	1.00	57.33	A
ATOM	499	CG	TRP	A	89	51.130	62.296	68.148	1.00	56.37	A
ATOM	500	CD2	TRP	A	89	52.229	62.998	67.571	1.00	56.15	A
ATOM	501	CE2	TRP	A	89	51.892	64.365	67.574	1.00	55.64	A
ATOM	502	CE3	TRP	A	89	53.463	62.605	67.044	1.00	55.77	A
ATOM	503	CD1	TRP	A	89	50.201	63.231	68.477	1.00	54.82	A
ATOM	504	NE1	TRP	A	89	50.649	64.480	68.136	1.00	54.93	A
ATOM	505	CZ2	TRP	A	89	52.755	65.342	67.072	1.00	55.82	A
ATOM	506	CZ3	TRP	A	89	54.315	63.579	66.544	1.00	55.23	A
ATOM	507	CH2	TRP	A	89	53.957	64.927	66.561	1.00	55.54	A
ATOM	508	C	TRP	A	89	50.915	60.332	65.831	1.00	57.32	A
ATOM	509	O	TRP	A	89	50.679	61.248	65.045	1.00	57.65	A
ATOM	510	N	ASP	A	90	51.827	59.398	65.593	1.00	55.46	A
ATOM	511	CA	ASP	A	90	52.602	59.387	64.366	1.00	53.21	A
ATOM	512	CB	ASP	A	90	53.710	58.353	64.472	1.00	51.45	A
ATOM	513	CG	ASP	A	90	54.795	58.795	65.396	1.00	51.44	A
ATOM	514	OD1	ASP	A	90	54.462	59.439	66.401	1.00	53.33	A
ATOM	515	OD2	ASP	A	90	55.975	58.511	65.134	1.00	51.16	A
ATOM	516	C	ASP	A	90	51.731	59.082	63.162	1.00	53.01	A
ATOM	517	O	ASP	A	90	51.943	59.625	62.076	1.00	53.15	A
ATOM	518	N	ARG	A	91	50.746	58.214	63.362	1.00	52.99	A
ATOM	519	CA	ARG	A	91	49.835	57.822	62.293	1.00	52.82	A
ATOM	520	CB	ARG	A	91	48.865	56.747	62.802	1.00	53.81	A
ATOM	521	CG	ARG	A	91	47.856	56.264	61.770	1.00	56.18	A
ATOM	522	CD	ARG	A	91	47.412	54.828	62.031	1.00	58.29	A
ATOM	523	NE	ARG	A	91	46.995	54.617	63.412	1.00	61.35	A
ATOM	524	CZ	ARG	A	91	45.922	55.168	63.972	1.00	62.36	A
ATOM	525	NH1	ARG	A	91	45.138	55.972	63.267	1.00	64.03	A
ATOM	526	NH2	ARG	A	91	45.640	54.925	65.246	1.00	63.29	A
ATOM	527	C	ARG	A	91	49.065	59.014	61.728	1.00	51.91	A
ATOM	528	O	ARG	A	91	48.829	59.086	60.522	1.00	51.24	A
ATOM	529	N	GLU	A	92	48.683	59.946	62.599	1.00	50.83	A
ATOM	530	CA	GLU	A	92	47.955	61.136	62.172	1.00	50.40	A
ATOM	531	CB	GLU	A	92	47.181	61.750	63.337	1.00	52.44	A
ATOM	532	CG	GLU	A	92	46.026	60.914	63.856	1.00	58.05	A
ATOM	533	CD	GLU	A	92	44.989	60.594	62.787	1.00	60.95	A
ATOM	534	OE1	GLU	A	92	44.493	61.541	62.125	1.00	61.85	A
ATOM	535	OE2	GLU	A	92	44.670	59.392	62.621	1.00	61.47	A
ATOM	536	C	GLU	A	92	48.929	62.174	61.632	1.00	48.17	A
ATOM	537	O	GLU	A	92	48.689	62.784	60.589	1.00	48.86	A

ATOM	538	N	PHE	A	93	50.020	62.376	62.364	1.00	45.11	A
ATOM	539	CA	PHE	A	93	51.056	63.325	61.989	1.00	42.22	A
ATOM	540	CB	PHE	A	93	52.241	63.197	62.930	1.00	39.86	A
ATOM	541	CG	PHE	A	93	53.473	63.881	62.431	1.00	38.61	A
ATOM	542	CD1	PHE	A	93	53.560	65.270	62.434	1.00	38.78	A
ATOM	543	CD2	PHE	A	93	54.550	63.139	61.949	1.00	38.41	A
ATOM	544	CE1	PHE	A	93	54.706	65.920	61.962	1.00	37.98	A
ATOM	545	CE2	PHE	A	93	55.702	63.771	61.474	1.00	37.53	A
ATOM	546	CZ	PHE	A	93	55.782	65.169	61.482	1.00	37.66	A
ATOM	547	C	PHE	A	93	51.529	63.039	60.586	1.00	41.92	A
ATOM	548	O	PHE	A	93	51.915	63.940	59.847	1.00	42.62	A
ATOM	549	N	LEU	A	94	51.513	61.766	60.229	1.00	41.18	A
ATOM	550	CA	LEU	A	94	51.938	61.368	58.913	1.00	40.65	A
ATOM	551	CB	LEU	A	94	52.602	60.008	58.986	1.00	39.81	A
ATOM	552	CG	LEU	A	94	53.987	60.082	59.611	1.00	40.12	A
ATOM	553	CD1	LEU	A	94	54.560	58.682	59.692	1.00	40.00	A
ATOM	554	CD2	LEU	A	94	54.889	60.998	58.785	1.00	38.29	A
ATOM	555	C	LEU	A	94	50.792	61.333	57.927	1.00	41.17	A
ATOM	556	O	LEU	A	94	51.010	61.120	56.737	1.00	41.27	A
ATOM	557	N	LYS	A	95	49.575	61.553	58.413	1.00	41.25	A
ATOM	558	CA	LYS	A	95	48.420	61.534	57.532	1.00	42.22	A
ATOM	559	CB	LYS	A	95	47.120	61.460	58.342	1.00	43.14	A
ATOM	560	CG	LYS	A	95	45.925	61.168	57.438	1.00	47.48	A
ATOM	561	CD	LYS	A	95	44.586	61.331	58.138	1.00	51.30	A
ATOM	562	CE	LYS	A	95	44.392	60.305	59.252	1.00	53.68	A
ATOM	563	NZ	LYS	A	95	43.042	60.431	59.895	1.00	54.53	A
ATOM	564	C	LYS	A	95	48.390	62.762	56.616	1.00	41.83	A
ATOM	565	O	LYS	A	95	47.450	63.552	56.650	1.00	42.87	A
ATOM	566	N	VAL	A	96	49.406	62.890	55.770	1.00	41.34	A
ATOM	567	CA	VAL	A	96	49.545	64.023	54.856	1.00	40.71	A
ATOM	568	CB	VAL	A	96	50.909	64.673	55.057	1.00	40.36	A
ATOM	569	CG1	VAL	A	96	51.034	65.180	56.471	1.00	39.98	A
ATOM	570	CG2	VAL	A	96	51.990	63.651	54.777	1.00	38.65	A
ATOM	571	C	VAL	A	96	49.446	63.611	53.385	1.00	41.10	A
ATOM	572	O	VAL	A	96	49.074	62.482	53.077	1.00	39.99	A
ATOM	573	N	ASP	A	97	49.789	64.518	52.471	1.00	41.74	A
ATOM	574	CA	ASP	A	97	49.729	64.155	51.064	1.00	43.35	A
ATOM	575	CB	ASP	A	97	49.500	65.386	50.168	1.00	46.03	A
ATOM	576	CG	ASP	A	97	50.694	66.307	50.088	1.00	49.27	A
ATOM	577	OD1	ASP	A	97	51.762	65.862	49.621	1.00	51.92	A
ATOM	578	OD2	ASP	A	97	50.560	67.490	50.476	1.00	50.75	A
ATOM	579	C	ASP	A	97	50.976	63.369	50.642	1.00	42.71	A
ATOM	580	O	ASP	A	97	52.039	63.493	51.249	1.00	42.39	A
ATOM	581	N	GLN	A	98	50.815	62.549	49.606	1.00	41.92	A
ATOM	582	CA	GLN	A	98	51.867	61.690	49.097	1.00	40.58	A
ATOM	583	CB	GLN	A	98	51.392	60.988	47.807	1.00	42.66	A
ATOM	584	CG	GLN	A	98	49.949	60.414	47.882	1.00	43.12	A
ATOM	585	CD	GLN	A	98	49.666	59.270	46.905	1.00	43.62	A
ATOM	586	OE1	GLN	A	98	48.516	58.876	46.720	1.00	42.97	A
ATOM	587	NE2	GLN	A	98	50.712	58.732	46.290	1.00	44.27	A
ATOM	588	C	GLN	A	98	53.173	62.428	48.870	1.00	39.89	A
ATOM	589	O	GLN	A	98	54.234	61.905	49.180	1.00	38.30	A
ATOM	590	N	GLU	A	99	53.114	63.640	48.330	1.00	40.88	A
ATOM	591	CA	GLU	A	99	54.343	64.404	48.118	1.00	40.74	A

```
ATOM    592  CB  GLU A  99      54.035  65.695  47.377  1.00 41.69      A
ATOM    593  CG  GLU A  99      53.880  65.494  45.903  1.00 47.00      A
ATOM    594  CD  GLU A  99      55.182  65.074  45.254  1.00 48.98      A
ATOM    595  OE1 GLU A  99      56.236  65.569  45.721  1.00 50.30      A
ATOM    596  OE2 GLU A  99      55.154  64.274  44.284  1.00 48.68      A
ATOM    597  C   GLU A  99      54.984  64.710  49.474  1.00 39.87      A
ATOM    598  O   GLU A  99      56.164  64.426  49.691  1.00 39.94      A
ATOM    599  N   MSE A 100      54.187  65.272  50.382  1.00 39.05      A
ATOM    600  CA  MSE A 100      54.637  65.617  51.729  1.00 39.03      A
ATOM    601  CB  MSE A 100      53.434  66.000  52.603  1.00 45.07      A
ATOM    602  CG  MSE A 100      53.726  66.188  54.093  1.00 50.78      A
ATOM    603  SE  MSE A 100      54.480  67.900  54.500  1.00 61.41      A
ATOM    604  CE  MSE A 100      56.351  67.467  54.330  1.00 55.82      A
ATOM    605  C   MSE A 100      55.366  64.446  52.371  1.00 36.07      A
ATOM    606  O   MSE A 100      56.517  64.561  52.789  1.00 34.98      A
ATOM    607  N   LEU A 101      54.681  63.316  52.436  1.00 32.38      A
ATOM    608  CA  LEU A 101      55.238  62.126  53.031  1.00 31.39      A
ATOM    609  CB  LEU A 101      54.241  60.993  52.880  1.00 30.22      A
ATOM    610  CG  LEU A 101      54.616  59.676  53.538  1.00 29.99      A
ATOM    611  CD1 LEU A 101      54.859  59.906  55.028  1.00 29.67      A
ATOM    612  CD2 LEU A 101      53.501  58.674  53.287  1.00 26.62      A
ATOM    613  C   LEU A 101      56.571  61.745  52.394  1.00 31.59      A
ATOM    614  O   LEU A 101      57.523  61.341  53.077  1.00 32.03      A
ATOM    615  N   TYR A 102      56.624  61.872  51.076  1.00 30.32      A
ATOM    616  CA  TYR A 102      57.814  61.556  50.311  1.00 29.70      A
ATOM    617  CB  TYR A 102      57.550  61.840  48.838  1.00 29.09      A
ATOM    618  CG  TYR A 102      58.765  61.747  47.940  1.00 27.92      A
ATOM    619  CD1 TYR A 102      59.402  60.530  47.709  1.00 27.22      A
ATOM    620  CE1 TYR A 102      60.478  60.441  46.831  1.00 27.22      A
ATOM    621  CD2 TYR A 102      59.243  62.873  47.274  1.00 26.92      A
ATOM    622  CE2 TYR A 102      60.314  62.792  46.401  1.00 24.90      A
ATOM    623  CZ  TYR A 102      60.921  61.580  46.181  1.00 26.49      A
ATOM    624  OH  TYR A 102      61.959  61.497  45.299  1.00 26.37      A
ATOM    625  C   TYR A 102      58.970  62.409  50.796  1.00 30.50      A
ATOM    626  O   TYR A 102      60.057  61.905  51.125  1.00 30.28      A
ATOM    627  N   GLU A 103      58.731  63.715  50.839  1.00 31.34      A
ATOM    628  CA  GLU A 103      59.763  64.645  51.276  1.00 32.16      A
ATOM    629  CB  GLU A 103      59.314  66.088  50.966  1.00 32.79      A
ATOM    630  CG  GLU A 103      58.921  66.251  49.492  1.00 35.11      A
ATOM    631  CD  GLU A 103      58.538  67.673  49.065  1.00 37.94      A
ATOM    632  OE1 GLU A 103      57.628  68.279  49.685  1.00 37.38      A
ATOM    633  OE2 GLU A 103      59.138  68.175  48.084  1.00 37.07      A
ATOM    634  C   GLU A 103      60.128  64.438  52.760  1.00 30.98      A
ATOM    635  O   GLU A 103      61.292  64.600  53.136  1.00 30.87      A
ATOM    636  N   ILE A 104      59.159  64.038  53.588  1.00 29.27      A
ATOM    637  CA  ILE A 104      59.426  63.804  55.011  1.00 28.70      A
ATOM    638  CB  ILE A 104      58.113  63.589  55.813  1.00 28.55      A
ATOM    639  CG2 ILE A 104      58.424  62.958  57.189  1.00 29.44      A
ATOM    640  CG1 ILE A 104      57.396  64.942  55.975  1.00 26.70      A
ATOM    641  CD1 ILE A 104      56.098  64.917  56.782  1.00 22.17      A
ATOM    642  C   ILE A 104      60.359  62.609  55.221  1.00 27.96      A
ATOM    643  O   ILE A 104      61.180  62.591  56.144  1.00 26.87      A
ATOM    644  N   ILE A 105      60.225  61.609  54.360  1.00 27.92      A
ATOM    645  CA  ILE A 105      61.082  60.439  54.435  1.00 26.71      A
```

ATOM	646	CB	ILE	A	105	60.543	59.321	53.534	1.00	26.61	A
ATOM	647	CG2	ILE	A	105	61.590	58.215	53.388	1.00	25.95	A
ATOM	648	CG1	ILE	A	105	59.200	58.836	54.106	1.00	26.49	A
ATOM	649	CD1	ILE	A	105	58.546	57.701	53.349	1.00	26.37	A
ATOM	650	C	ILE	A	105	62.500	60.825	54.017	1.00	26.46	A
ATOM	651	O	ILE	A	105	63.484	60.401	54.639	1.00	26.10	A
ATOM	652	N	LEU	A	106	62.603	61.648	52.975	1.00	25.01	A
ATOM	653	CA	LEU	A	106	63.915	62.084	52.505	1.00	24.17	A
ATOM	654	CB	LEU	A	106	63.802	62.917	51.230	1.00	23.30	A
ATOM	655	CG	LEU	A	106	63.211	62.283	49.961	1.00	22.86	A
ATOM	656	CD1	LEU	A	106	63.415	63.252	48.829	1.00	19.46	A
ATOM	657	CD2	LEU	A	106	63.875	60.950	49.639	1.00	17.99	A
ATOM	658	C	LEU	A	106	64.612	62.904	53.574	1.00	24.05	A
ATOM	659	O	LEU	A	106	65.792	62.701	53.860	1.00	24.80	A
ATOM	660	N	ALA	A	107	63.875	63.835	54.168	1.00	23.58	A
ATOM	661	CA	ALA	A	107	64.430	64.676	55.218	1.00	23.64	A
ATOM	662	CB	ALA	A	107	63.388	65.684	55.684	1.00	21.11	A
ATOM	663	C	ALA	A	107	64.901	63.817	56.393	1.00	23.90	A
ATOM	664	O	ALA	A	107	65.978	64.046	56.952	1.00	23.39	A
ATOM	665	N	ALA	A	108	64.093	62.838	56.779	1.00	24.83	A
ATOM	666	CA	ALA	A	108	64.479	61.970	57.879	1.00	27.43	A
ATOM	667	CB	ALA	A	108	63.343	60.984	58.215	1.00	27.65	A
ATOM	668	C	ALA	A	108	65.727	61.211	57.456	1.00	28.80	A
ATOM	669	O	ALA	A	108	66.646	61.009	58.249	1.00	29.92	A
ATOM	670	N	ASN	A	109	65.763	60.794	56.196	1.00	28.89	A
ATOM	671	CA	ASN	A	109	66.920	60.062	55.719	1.00	29.68	A
ATOM	672	CB	ASN	A	109	66.631	59.416	54.361	1.00	31.27	A
ATOM	673	CG	ASN	A	109	67.744	58.480	53.915	1.00	31.80	A
ATOM	674	OD1	ASN	A	109	68.755	58.912	53.362	1.00	31.60	A
ATOM	675	ND2	ASN	A	109	67.568	57.186	54.178	1.00	32.93	A
ATOM	676	C	ASN	A	109	68.153	60.956	55.628	1.00	30.29	A
ATOM	677	O	ASN	A	109	69.248	60.524	55.959	1.00	30.81	A
ATOM	678	N	TYR	A	110	67.992	62.197	55.177	1.00	31.42	A
ATOM	679	CA	TYR	A	110	69.133	63.105	55.080	1.00	31.10	A
ATOM	680	CB	TYR	A	110	68.756	64.363	54.312	1.00	29.98	A
ATOM	681	CG	TYR	A	110	69.819	65.437	54.351	1.00	30.69	A
ATOM	682	CD1	TYR	A	110	71.057	65.237	53.736	1.00	29.71	A
ATOM	683	CE1	TYR	A	110	72.022	66.241	53.716	1.00	30.17	A
ATOM	684	CD2	TYR	A	110	69.571	66.674	54.965	1.00	31.52	A
ATOM	685	CE2	TYR	A	110	70.526	67.686	54.954	1.00	31.71	A
ATOM	686	CZ	TYR	A	110	71.750	67.463	54.318	1.00	32.53	A
ATOM	687	OH	TYR	A	110	72.680	68.481	54.226	1.00	33.63	A
ATOM	688	C	TYR	A	110	69.620	63.515	56.463	1.00	31.73	A
ATOM	689	O	TYR	A	110	70.818	63.603	56.694	1.00	32.81	A
ATOM	690	N	LEU	A	111	68.682	63.770	57.371	1.00	30.92	A
ATOM	691	CA	LEU	A	111	69.016	64.184	58.719	1.00	31.21	A
ATOM	692	CB	LEU	A	111	67.870	64.994	59.317	1.00	28.89	A
ATOM	693	CG	LEU	A	111	67.630	66.380	58.734	1.00	26.61	A
ATOM	694	CD1	LEU	A	111	66.251	66.831	59.141	1.00	24.78	A
ATOM	695	CD2	LEU	A	111	68.694	67.360	59.200	1.00	24.10	A
ATOM	696	C	LEU	A	111	69.337	63.006	59.624	1.00	33.12	A
ATOM	697	O	LEU	A	111	69.590	63.181	60.816	1.00	34.02	A
ATOM	698	N	ASN	A	112	69.319	61.805	59.062	1.00	33.71	A
ATOM	699	CA	ASN	A	112	69.620	60.588	59.820	1.00	34.83	A

```
ATOM    700  CB  ASN A 112      71.102  60.570  60.204  1.00 33.95      A
ATOM    701  CG  ASN A 112      71.644  59.164  60.365  1.00 33.26      A
ATOM    702  OD1 ASN A 112      71.015  58.322  60.977  1.00 34.03      A
ATOM    703  ND2 ASN A 112      72.820  58.913  59.813  1.00 34.72      A
ATOM    704  C   ASN A 112      68.764  60.460  61.091  1.00 35.67      A
ATOM    705  O   ASN A 112      69.272  60.582  62.209  1.00 37.75      A
ATOM    706  N   ILE A 113      67.472  60.203  60.906  1.00 35.48      A
ATOM    707  CA  ILE A 113      66.517  60.055  62.005  1.00 35.39      A
ATOM    708  CB  ILE A 113      65.531  61.253  62.034  1.00 35.97      A
ATOM    709  CG2 ILE A 113      64.563  61.125  63.200  1.00 35.08      A
ATOM    710  CG1 ILE A 113      66.307  62.567  62.154  1.00 36.19      A
ATOM    711  CD1 ILE A 113      65.427  63.795  62.132  1.00 33.68      A
ATOM    712  C   ILE A 113      65.738  58.761  61.763  1.00 35.67      A
ATOM    713  O   ILE A 113      64.564  58.789  61.381  1.00 33.98      A
ATOM    714  N   LYS A 114      66.408  57.632  61.988  1.00 37.77      A
ATOM    715  CA  LYS A 114      65.827  56.299  61.775  1.00 39.09      A
ATOM    716  CB  LYS A 114      66.697  55.238  62.461  1.00 41.82      A
ATOM    717  CG  LYS A 114      67.835  54.703  61.601  1.00 45.96      A
ATOM    718  CD  LYS A 114      68.786  55.789  61.081  1.00 47.81      A
ATOM    719  CE  LYS A 114      69.952  55.145  60.306  1.00 49.70      A
ATOM    720  NZ  LYS A 114      69.498  54.249  59.161  1.00 51.87      A
ATOM    721  C   LYS A 114      64.372  56.128  62.216  1.00 37.68      A
ATOM    722  O   LYS A 114      63.521  55.697  61.438  1.00 38.17      A
ATOM    723  N   PRO A 115      64.076  56.435  63.484  1.00 36.13      A
ATOM    724  CD  PRO A 115      65.015  56.886  64.526  1.00 34.15      A
ATOM    725  CA  PRO A 115      62.715  56.314  64.011  1.00 34.44      A
ATOM    726  CB  PRO A 115      62.815  57.022  65.351  1.00 34.06      A
ATOM    727  CG  PRO A 115      64.220  56.680  65.777  1.00 35.33      A
ATOM    728  C   PRO A 115      61.694  56.968  63.076  1.00 33.56      A
ATOM    729  O   PRO A 115      60.658  56.384  62.763  1.00 33.50      A
ATOM    730  N   LEU A 116      62.001  58.179  62.622  1.00 31.71      A
ATOM    731  CA  LEU A 116      61.108  58.903  61.733  1.00 30.40      A
ATOM    732  CB  LEU A 116      61.583  60.347  61.567  1.00 29.42      A
ATOM    733  CG  LEU A 116      60.603  61.229  60.796  1.00 28.24      A
ATOM    734  CD1 LEU A 116      59.268  61.223  61.507  1.00 28.18      A
ATOM    735  CD2 LEU A 116      61.144  62.633  60.674  1.00 29.52      A
ATOM    736  C   LEU A 116      61.005  58.211  60.375  1.00 30.54      A
ATOM    737  O   LEU A 116      59.909  58.046  59.823  1.00 29.43      A
ATOM    738  N   LEU A 117      62.150  57.804  59.836  1.00 30.80      A
ATOM    739  CA  LEU A 117      62.193  57.097  58.555  1.00 30.78      A
ATOM    740  CB  LEU A 117      63.632  56.678  58.223  1.00 28.60      A
ATOM    741  CG  LEU A 117      63.843  55.833  56.966  1.00 27.90      A
ATOM    742  CD1 LEU A 117      63.388  56.587  55.756  1.00 26.40      A
ATOM    743  CD2 LEU A 117      65.304  55.467  56.830  1.00 29.33      A
ATOM    744  C   LEU A 117      61.311  55.856  58.624  1.00 32.57      A
ATOM    745  O   LEU A 117      60.403  55.675  57.800  1.00 33.66      A
ATOM    746  N   ASP A 118      61.588  55.002  59.608  1.00 32.30      A
ATOM    747  CA  ASP A 118      60.821  53.781  59.777  1.00 32.82      A
ATOM    748  CB  ASP A 118      61.241  53.035  61.046  1.00 34.51      A
ATOM    749  CG  ASP A 118      62.660  52.481  60.958  1.00 38.01      A
ATOM    750  OD1 ASP A 118      63.075  52.088  59.841  1.00 37.92      A
ATOM    751  OD2 ASP A 118      63.355  52.432  62.007  1.00 38.31      A
ATOM    752  C   ASP A 118      59.345  54.104  59.836  1.00 32.67      A
ATOM    753  O   ASP A 118      58.533  53.458  59.160  1.00 33.71      A
```

```
ATOM    754  N   ALA A 119      58.997  55.109  60.632  1.00 31.48      A
ATOM    755  CA  ALA A 119      57.600  55.512  60.774  1.00 32.03      A
ATOM    756  CB  ALA A 119      57.512  56.753  61.625  1.00 31.77      A
ATOM    757  C   ALA A 119      56.961  55.774  59.418  1.00 32.00      A
ATOM    758  O   ALA A 119      55.932  55.185  59.071  1.00 31.09      A
ATOM    759  N   GLY A 120      57.582  56.673  58.660  1.00 32.93      A
ATOM    760  CA  GLY A 120      57.081  57.007  57.341  1.00 33.63      A
ATOM    761  C   GLY A 120      57.019  55.773  56.469  1.00 33.78      A
ATOM    762  O   GLY A 120      56.045  55.571  55.748  1.00 33.76      A
ATOM    763  N   CYS A 121      58.056  54.944  56.522  1.00 34.09      A
ATOM    764  CA  CYS A 121      58.048  53.735  55.714  1.00 37.06      A
ATOM    765  CB  CYS A 121      59.370  52.985  55.852  1.00 37.59      A
ATOM    766  SG  CYS A 121      60.672  53.684  54.825  1.00 37.93      A
ATOM    767  C   CYS A 121      56.882  52.814  56.063  1.00 36.49      A
ATOM    768  O   CYS A 121      56.222  52.272  55.177  1.00 37.36      A
ATOM    769  N   LYS A 122      56.617  52.645  57.348  1.00 36.54      A
ATOM    770  CA  LYS A 122      55.525  51.786  57.766  1.00 37.44      A
ATOM    771  CB  LYS A 122      55.445  51.751  59.288  1.00 38.22      A
ATOM    772  CG  LYS A 122      56.652  51.150  59.950  1.00 38.67      A
ATOM    773  CD  LYS A 122      56.424  51.081  61.441  1.00 42.04      A
ATOM    774  CE  LYS A 122      57.663  50.592  62.185  1.00 42.25      A
ATOM    775  NZ  LYS A 122      57.394  50.419  63.636  1.00 41.74      A
ATOM    776  C   LYS A 122      54.197  52.276  57.208  1.00 36.82      A
ATOM    777  O   LYS A 122      53.340  51.479  56.812  1.00 36.50      A
ATOM    778  N   VAL A 123      54.035  53.595  57.187  1.00 36.30      A
ATOM    779  CA  VAL A 123      52.810  54.208  56.699  1.00 35.72      A
ATOM    780  CB  VAL A 123      52.832  55.718  56.967  1.00 36.26      A
ATOM    781  CG1 VAL A 123      51.483  56.319  56.621  1.00 36.90      A
ATOM    782  CG2 VAL A 123      53.170  55.966  58.429  1.00 35.63      A
ATOM    783  C   VAL A 123      52.576  53.929  55.208  1.00 35.46      A
ATOM    784  O   VAL A 123      51.448  53.633  54.793  1.00 33.96      A
ATOM    785  N   VAL A 124      53.639  54.007  54.406  1.00 35.31      A
ATOM    786  CA  VAL A 124      53.510  53.737  52.970  1.00 34.89      A
ATOM    787  CB  VAL A 124      54.815  54.026  52.177  1.00 34.43      A
ATOM    788  CG1 VAL A 124      54.564  53.832  50.682  1.00 32.55      A
ATOM    789  CG2 VAL A 124      55.294  55.442  52.449  1.00 34.56      A
ATOM    790  C   VAL A 124      53.135  52.273  52.767  1.00 34.07      A
ATOM    791  O   VAL A 124      52.317  51.947  51.898  1.00 34.52      A
ATOM    792  N   ALA A 125      53.734  51.401  53.575  1.00 32.52      A
ATOM    793  CA  ALA A 125      53.452  49.974  53.500  1.00 33.46      A
ATOM    794  CB  ALA A 125      54.294  49.221  54.496  1.00 31.49      A
ATOM    795  C   ALA A 125      51.975  49.757  53.805  1.00 35.59      A
ATOM    796  O   ALA A 125      51.283  48.987  53.127  1.00 35.62      A
ATOM    797  N   GLU A 126      51.495  50.462  54.823  1.00 37.35      A
ATOM    798  CA  GLU A 126      50.107  50.357  55.213  1.00 37.88      A
ATOM    799  CB  GLU A 126      49.864  51.130  56.494  1.00 39.94      A
ATOM    800  CG  GLU A 126      50.589  50.522  57.658  1.00 44.44      A
ATOM    801  CD  GLU A 126      49.884  50.789  58.974  1.00 47.25      A
ATOM    802  OE1 GLU A 126      49.926  51.949  59.454  1.00 46.76      A
ATOM    803  OE2 GLU A 126      49.271  49.832  59.516  1.00 49.61      A
ATOM    804  C   GLU A 126      49.149  50.812  54.142  1.00 37.12      A
ATOM    805  O   GLU A 126      47.974  50.472  54.189  1.00 36.85      A
ATOM    806  N   MSE A 127      49.648  51.573  53.176  1.00 37.83      A
ATOM    807  CA  MSE A 127      48.814  52.035  52.085  1.00 38.50      A
```

```
ATOM    808  CB  MSE A 127      49.473  53.225  51.396  1.00 39.64      A
ATOM    809  CG  MSE A 127      49.682  54.471  52.264  1.00 40.86      A
ATOM    810  SE  MSE A 127      50.428  55.994  51.160  1.00 44.01      A
ATOM    811  CE  MSE A 127      48.774  56.477  50.261  1.00 43.47      A
ATOM    812  C   MSE A 127      48.621  50.885  51.092  1.00 38.76      A
ATOM    813  O   MSE A 127      47.586  50.792  50.443  1.00 38.95      A
ATOM    814  N   ILE A 128      49.607  49.997  51.003  1.00 39.74      A
ATOM    815  CA  ILE A 128      49.552  48.849  50.090  1.00 40.70      A
ATOM    816  CB  ILE A 128      50.989  48.359  49.755  1.00 39.21      A
ATOM    817  CG2 ILE A 128      50.935  47.158  48.828  1.00 39.17      A
ATOM    818  CG1 ILE A 128      51.797  49.518  49.163  1.00 37.59      A
ATOM    819  CD1 ILE A 128      53.148  49.159  48.595  1.00 35.03      A
ATOM    820  C   ILE A 128      48.777  47.698  50.736  1.00 42.24      A
ATOM    821  O   ILE A 128      47.886  47.098  50.132  1.00 40.92      A
ATOM    822  N   ARG A 129      49.147  47.412  51.980  1.00 46.16      A
ATOM    823  CA  ARG A 129      48.556  46.350  52.792  1.00 49.18      A
ATOM    824  CB  ARG A 129      48.696  46.701  54.268  1.00 50.29      A
ATOM    825  CG  ARG A 129      48.224  45.614  55.205  1.00 53.92      A
ATOM    826  CD  ARG A 129      48.566  45.978  56.643  1.00 58.68      A
ATOM    827  NE  ARG A 129      49.936  46.490  56.743  1.00 62.87      A
ATOM    828  CZ  ARG A 129      50.553  46.798  57.881  1.00 64.32      A
ATOM    829  NH1 ARG A 129      49.927  46.647  59.045  1.00 64.82      A
ATOM    830  NH2 ARG A 129      51.799  47.258  57.850  1.00 64.62      A
ATOM    831  C   ARG A 129      47.094  46.044  52.498  1.00 49.27      A
ATOM    832  O   ARG A 129      46.230  46.920  52.589  1.00 49.24      A
ATOM    833  N   GLY A 130      46.839  44.785  52.158  1.00 48.73      A
ATOM    834  CA  GLY A 130      45.492  44.354  51.873  1.00 49.33      A
ATOM    835  C   GLY A 130      44.843  44.937  50.632  1.00 50.07      A
ATOM    836  O   GLY A 130      43.619  44.856  50.486  1.00 49.22      A
ATOM    837  N   ARG A 131      45.630  45.523  49.735  1.00 49.98      A
ATOM    838  CA  ARG A 131      45.048  46.086  48.524  1.00 50.73      A
ATOM    839  CB  ARG A 131      45.402  47.573  48.410  1.00 51.87      A
ATOM    840  CG  ARG A 131      44.801  48.429  49.545  1.00 54.75      A
ATOM    841  CD  ARG A 131      45.035  49.929  49.340  1.00 57.52      A
ATOM    842  NE  ARG A 131      44.412  50.438  48.116  1.00 60.43      A
ATOM    843  CZ  ARG A 131      43.098  50.531  47.910  1.00 61.10      A
ATOM    844  NH1 ARG A 131      42.248  50.147  48.855  1.00 60.79      A
ATOM    845  NH2 ARG A 131      42.634  51.009  46.755  1.00 61.77      A
ATOM    846  C   ARG A 131      45.447  45.325  47.261  1.00 50.69      A
ATOM    847  O   ARG A 131      46.432  44.592  47.249  1.00 51.15      A
ATOM    848  N   SER A 132      44.670  45.494  46.199  1.00 50.35      A
ATOM    849  CA  SER A 132      44.941  44.798  44.950  1.00 50.32      A
ATOM    850  CB  SER A 132      43.630  44.489  44.224  1.00 49.61      A
ATOM    851  OG  SER A 132      43.082  45.662  43.648  1.00 48.59      A
ATOM    852  C   SER A 132      45.837  45.608  44.023  1.00 50.87      A
ATOM    853  O   SER A 132      46.056  46.808  44.235  1.00 50.23      A
ATOM    854  N   PRO A 133      46.359  44.957  42.970  1.00 50.57      A
ATOM    855  CD  PRO A 133      46.253  43.520  42.659  1.00 49.65      A
ATOM    856  CA  PRO A 133      47.230  45.628  42.006  1.00 50.93      A
ATOM    857  CB  PRO A 133      47.392  44.581  40.914  1.00 50.37      A
ATOM    858  CG  PRO A 133      47.405  43.315  41.698  1.00 50.36      A
ATOM    859  C   PRO A 133      46.616  46.915  41.483  1.00 51.56      A
ATOM    860  O   PRO A 133      47.263  47.964  41.480  1.00 52.20      A
ATOM    861  N   GLU A 134      45.364  46.839  41.044  1.00 51.94      A
```

```
ATOM    862  CA  GLU A 134      44.693  48.021  40.516  1.00 52.22      A
ATOM    863  CB  GLU A 134      43.395  47.637  39.811  1.00 54.08      A
ATOM    864  CG  GLU A 134      43.436  47.886  38.314  1.00 58.97      A
ATOM    865  CD  GLU A 134      43.821  49.320  37.974  1.00 62.39      A
ATOM    866  OE1 GLU A 134      43.122  50.254  38.436  1.00 63.15      A
ATOM    867  OE2 GLU A 134      44.823  49.513  37.243  1.00 64.67      A
ATOM    868  C   GLU A 134      44.406  49.035  41.610  1.00 50.15      A
ATOM    869  O   GLU A 134      44.400  50.244  41.355  1.00 49.58      A
ATOM    870  N   GLU A 135      44.177  48.539  42.823  1.00 47.26      A
ATOM    871  CA  GLU A 135      43.904  49.412  43.948  1.00 45.19      A
ATOM    872  CB  GLU A 135      43.390  48.613  45.142  1.00 44.69      A
ATOM    873  CG  GLU A 135      41.973  48.135  44.948  1.00 47.13      A
ATOM    874  CD  GLU A 135      41.333  47.585  46.207  1.00 49.00      A
ATOM    875  OE1 GLU A 135      41.857  46.590  46.766  1.00 49.49      A
ATOM    876  OE2 GLU A 135      40.295  48.153  46.633  1.00 50.00      A
ATOM    877  C   GLU A 135      45.160  50.162  44.328  1.00 43.66      A
ATOM    878  O   GLU A 135      45.113  51.349  44.650  1.00 42.57      A
ATOM    879  N   ILE A 136      46.288  49.467  44.269  1.00 41.78      A
ATOM    880  CA  ILE A 136      47.558  50.077  44.622  1.00 41.23      A
ATOM    881  CB  ILE A 136      48.646  49.014  44.782  1.00 39.22      A
ATOM    882  CG2 ILE A 136      49.957  49.675  45.197  1.00 37.75      A
ATOM    883  CG1 ILE A 136      48.180  47.970  45.801  1.00 37.01      A
ATOM    884  CD1 ILE A 136      49.154  46.847  46.033  1.00 34.37      A
ATOM    885  C   ILE A 136      47.993  51.065  43.558  1.00 42.50      A
ATOM    886  O   ILE A 136      48.490  52.162  43.856  1.00 42.93      A
ATOM    887  N   ARG A 137      47.787  50.651  42.314  1.00 42.34      A
ATOM    888  CA  ARG A 137      48.144  51.439  41.151  1.00 41.82      A
ATOM    889  CB  ARG A 137      47.844  50.636  39.884  1.00 42.65      A
ATOM    890  CG  ARG A 137      48.949  50.635  38.849  1.00 43.90      A
ATOM    891  CD  ARG A 137      48.594  49.715  37.679  1.00 45.63      A
ATOM    892  NE  ARG A 137      48.503  48.315  38.092  1.00 47.76      A
ATOM    893  CZ  ARG A 137      47.567  47.477  37.664  1.00 48.21      A
ATOM    894  NH1 ARG A 137      46.644  47.901  36.810  1.00 49.10      A
ATOM    895  NH2 ARG A 137      47.546  46.226  38.099  1.00 48.10      A
ATOM    896  C   ARG A 137      47.348  52.736  41.156  1.00 40.67      A
ATOM    897  O   ARG A 137      47.821  53.773  40.685  1.00 39.93      A
ATOM    898  N   ARG A 138      46.134  52.677  41.694  1.00 40.67      A
ATOM    899  CA  ARG A 138      45.276  53.864  41.756  1.00 40.88      A
ATOM    900  CB  ARG A 138      43.807  53.456  41.932  1.00 39.95      A
ATOM    901  CG  ARG A 138      43.140  52.934  40.660  0.00 41.86      A
ATOM    902  CD  ARG A 138      43.070  53.989  39.550  0.00 42.76      A
ATOM    903  NE  ARG A 138      44.301  54.072  38.764  0.00 43.72      A
ATOM    904  CZ  ARG A 138      44.443  54.802  37.659  0.00 44.10      A
ATOM    905  NH1 ARG A 138      43.430  55.523  37.196  0.00 44.35      A
ATOM    906  NH2 ARG A 138      45.602  54.812  37.015  0.00 44.35      A
ATOM    907  C   ARG A 138      45.706  54.791  42.895  1.00 39.80      A
ATOM    908  O   ARG A 138      45.705  56.016  42.762  1.00 39.09      A
ATOM    909  N   THR A 139      46.083  54.177  44.008  1.00 39.87      A
ATOM    910  CA  THR A 139      46.544  54.877  45.193  1.00 39.93      A
ATOM    911  CB  THR A 139      47.058  53.872  46.234  1.00 40.30      A
ATOM    912  OG1 THR A 139      45.971  53.054  46.689  1.00 40.58      A
ATOM    913  CG2 THR A 139      47.684  54.602  47.420  1.00 41.79      A
ATOM    914  C   THR A 139      47.674  55.849  44.881  1.00 41.13      A
ATOM    915  O   THR A 139      47.752  56.941  45.455  1.00 42.14      A
```

ATOM	916	N	PHE	A	140	48.559	55.443	43.978	1.00	41.08	A
ATOM	917	CA	PHE	A	140	49.705	56.267	43.607	1.00	39.57	A
ATOM	918	CB	PHE	A	140	50.986	55.449	43.755	1.00	38.91	A
ATOM	919	CG	PHE	A	140	51.220	54.943	45.145	1.00	38.38	A
ATOM	920	CD1	PHE	A	140	51.519	55.824	46.174	1.00	38.13	A
ATOM	921	CD2	PHE	A	140	51.122	53.588	45.432	1.00	37.94	A
ATOM	922	CE1	PHE	A	140	51.722	55.364	47.464	1.00	38.18	A
ATOM	923	CE2	PHE	A	140	51.323	53.118	46.721	1.00	37.42	A
ATOM	924	CZ	PHE	A	140	51.622	54.008	47.739	1.00	38.51	A
ATOM	925	C	PHE	A	140	49.600	56.779	42.185	1.00	39.01	A
ATOM	926	O	PHE	A	140	50.512	57.434	41.685	1.00	39.06	A
ATOM	927	N	ASN	A	141	48.485	56.483	41.537	1.00	38.54	A
ATOM	928	CA	ASN	A	141	48.294	56.894	40.162	1.00	38.58	A
ATOM	929	CB	ASN	A	141	48.220	58.407	40.049	1.00	39.46	A
ATOM	930	CG	ASN	A	141	47.787	58.847	38.669	1.00	41.82	A
ATOM	931	OD1	ASN	A	141	46.655	58.592	38.257	1.00	44.53	A
ATOM	932	ND2	ASN	A	141	48.687	59.495	37.938	1.00	42.34	A
ATOM	933	C	ASN	A	141	49.439	56.378	39.296	1.00	38.74	A
ATOM	934	O	ASN	A	141	50.031	57.122	38.503	1.00	38.59	A
ATOM	935	N	ILE	A	142	49.738	55.093	39.459	1.00	38.05	A
ATOM	936	CA	ILE	A	142	50.800	54.429	38.715	1.00	37.68	A
ATOM	937	CB	ILE	A	142	51.425	53.321	39.561	1.00	36.00	A
ATOM	938	CG2	ILE	A	142	52.451	52.563	38.755	1.00	34.95	A
ATOM	939	CG1	ILE	A	142	52.021	53.921	40.829	1.00	35.82	A
ATOM	940	CD1	ILE	A	142	52.449	52.875	41.837	1.00	36.82	A
ATOM	941	C	ILE	A	142	50.239	53.819	37.440	1.00	38.81	A
ATOM	942	O	ILE	A	142	49.121	53.321	37.441	1.00	39.45	A
ATOM	943	N	VAL	A	143	51.022	53.855	36.361	1.00	40.31	A
ATOM	944	CA	VAL	A	143	50.620	53.310	35.053	1.00	40.27	A
ATOM	945	CB	VAL	A	143	51.373	54.017	33.905	1.00	42.11	A
ATOM	946	CG1	VAL	A	143	51.035	53.348	32.567	1.00	42.72	A
ATOM	947	CG2	VAL	A	143	51.016	55.493	33.877	1.00	41.43	A
ATOM	948	C	VAL	A	143	50.868	51.808	34.881	1.00	39.19	A
ATOM	949	O	VAL	A	143	51.955	51.309	35.172	1.00	38.15	A
ATOM	950	N	ASN	A	144	49.869	51.107	34.359	1.00	38.94	A
ATOM	951	CA	ASN	A	144	49.968	49.670	34.137	1.00	39.16	A
ATOM	952	CB	ASN	A	144	48.575	49.048	34.256	1.00	39.51	A
ATOM	953	CG	ASN	A	144	48.570	47.573	33.959	1.00	40.78	A
ATOM	954	OD1	ASN	A	144	49.586	46.903	34.090	1.00	44.00	A
ATOM	955	ND2	ASN	A	144	47.421	47.052	33.574	1.00	41.05	A
ATOM	956	C	ASN	A	144	50.582	49.341	32.775	1.00	38.55	A
ATOM	957	O	ASN	A	144	49.876	48.975	31.839	1.00	37.91	A
ATOM	958	N	ASP	A	145	51.902	49.448	32.685	1.00	38.25	A
ATOM	959	CA	ASP	A	145	52.624	49.190	31.440	1.00	39.85	A
ATOM	960	CB	ASP	A	145	53.996	49.862	31.498	1.00	39.46	A
ATOM	961	CG	ASP	A	145	54.766	49.490	32.750	1.00	39.69	A
ATOM	962	OD1	ASP	A	145	54.213	48.735	33.587	1.00	39.21	A
ATOM	963	OD2	ASP	A	145	55.918	49.947	32.895	1.00	38.21	A
ATOM	964	C	ASP	A	145	52.798	47.712	31.092	1.00	40.13	A
ATOM	965	O	ASP	A	145	53.702	47.343	30.337	1.00	39.56	A
ATOM	966	N	PHE	A	146	51.938	46.870	31.652	1.00	40.47	A
ATOM	967	CA	PHE	A	146	51.978	45.440	31.377	1.00	40.10	A
ATOM	968	CB	PHE	A	146	51.371	44.644	32.541	1.00	39.31	A
ATOM	969	CG	PHE	A	146	52.301	44.453	33.699	1.00	40.02	A

```
ATOM    970  CD1 PHE A 146      53.534  43.850  33.520  1.00 39.21      A
ATOM    971  CD2 PHE A 146      51.952  44.889  34.971  1.00 39.97      A
ATOM    972  CE1 PHE A 146      54.407  43.690  34.591  1.00 39.41      A
ATOM    973  CE2 PHE A 146      52.827  44.731  36.051  1.00 38.93      A
ATOM    974  CZ  PHE A 146      54.053  44.131  35.858  1.00 38.17      A
ATOM    975  C   PHE A 146      51.167  45.171  30.113  1.00 40.82      A
ATOM    976  O   PHE A 146      50.013  45.603  29.999  1.00 41.89      A
ATOM    977  N   THR A 147      51.773  44.476  29.154  1.00 40.38      A
ATOM    978  CA  THR A 147      51.073  44.137  27.922  1.00 38.81      A
ATOM    979  CB  THR A 147      51.999  43.509  26.877  1.00 38.98      A
ATOM    980  OG1 THR A 147      52.651  42.373  27.456  1.00 39.24      A
ATOM    981  CG2 THR A 147      53.030  44.498  26.395  1.00 36.50      A
ATOM    982  C   THR A 147      50.062  43.070  28.286  1.00 38.78      A
ATOM    983  O   THR A 147      50.233  42.343  29.268  1.00 37.08      A
ATOM    984  N   PRO A 148      49.003  42.943  27.485  1.00 39.53      A
ATOM    985  CD  PRO A 148      48.718  43.722  26.266  1.00 39.08      A
ATOM    986  CA  PRO A 148      47.958  41.947  27.732  1.00 40.59      A
ATOM    987  CB  PRO A 148      47.166  41.970  26.428  1.00 39.52      A
ATOM    988  CG  PRO A 148      47.260  43.419  26.034  1.00 39.40      A
ATOM    989  C   PRO A 148      48.505  40.545  28.078  1.00 42.69      A
ATOM    990  O   PRO A 148      48.007  39.876  28.984  1.00 43.05      A
ATOM    991  N   GLU A 149      49.546  40.123  27.370  1.00 45.32      A
ATOM    992  CA  GLU A 149      50.155  38.814  27.572  1.00 46.47      A
ATOM    993  CB  GLU A 149      51.059  38.496  26.395  1.00 44.18      A
ATOM    994  CG  GLU A 149      51.681  37.137  26.430  1.00 43.56      A
ATOM    995  CD  GLU A 149      52.660  36.955  25.311  1.00 43.86      A
ATOM    996  OE1 GLU A 149      53.660  37.699  25.279  1.00 43.12      A
ATOM    997  OE2 GLU A 149      52.430  36.075  24.458  1.00 44.44      A
ATOM    998  C   GLU A 149      50.974  38.773  28.845  1.00 48.79      A
ATOM    999  O   GLU A 149      50.852  37.856  29.660  1.00 49.11      A
ATOM   1000  N   GLU A 150      51.826  39.773  29.006  1.00 52.88      A
ATOM   1001  CA  GLU A 150      52.676  39.855  30.180  1.00 56.79      A
ATOM   1002  CB  GLU A 150      53.548  41.105  30.090  1.00 56.56      A
ATOM   1003  CG  GLU A 150      54.707  41.109  31.045  1.00 57.96      A
ATOM   1004  CD  GLU A 150      55.774  40.103  30.660  1.00 59.33      A
ATOM   1005  OE1 GLU A 150      55.489  38.887  30.639  1.00 60.34      A
ATOM   1006  OE2 GLU A 150      56.907  40.533  30.372  1.00 60.87      A
ATOM   1007  C   GLU A 150      51.804  39.913  31.433  1.00 59.23      A
ATOM   1008  O   GLU A 150      52.187  39.417  32.488  1.00 59.36      A
ATOM   1009  N   GLU A 151      50.627  40.519  31.305  1.00 62.33      A
ATOM   1010  CA  GLU A 151      49.701  40.651  32.424  1.00 64.96      A
ATOM   1011  CB  GLU A 151      48.477  41.452  31.982  1.00 65.44      A
ATOM   1012  CG  GLU A 151      48.102  42.579  32.923  1.00 66.38      A
ATOM   1013  CD  GLU A 151      47.141  43.563  32.287  1.00 67.52      A
ATOM   1014  OE1 GLU A 151      47.510  44.187  31.269  1.00 67.49      A
ATOM   1015  OE2 GLU A 151      46.014  43.713  32.803  1.00 68.18      A
ATOM   1016  C   GLU A 151      49.270  39.286  32.954  1.00 66.62      A
ATOM   1017  O   GLU A 151      49.543  38.943  34.104  1.00 66.87      A
ATOM   1018  N   ALA A 152      48.602  38.512  32.106  1.00 68.29      A
ATOM   1019  CA  ALA A 152      48.137  37.181  32.474  1.00 70.15      A
ATOM   1020  CB  ALA A 152      47.511  36.503  31.268  1.00 70.09      A
ATOM   1021  C   ALA A 152      49.280  36.327  33.014  1.00 71.79      A
ATOM   1022  O   ALA A 152      49.085  35.503  33.903  1.00 71.18      A
ATOM   1023  N   ALA A 153      50.477  36.526  32.475  1.00 74.38      A
```

	ATOM	1024	CA	ALA	A	153	51.632	35.761	32.917	1.00	76.96	A
	ATOM	1025	CB	ALA	A	153	52.834	36.056	32.020	1.00	76.52	A
	ATOM	1026	C	ALA	A	153	51.969	36.069	34.376	1.00	79.23	A
	ATOM	1027	O	ALA	A	153	53.040	35.700	34.863	1.00	80.18	A
5	ATOM	1028	N	ILE	A	154	51.061	36.759	35.067	1.00	80.86	A
	ATOM	1029	CA	ILE	A	154	51.257	37.103	36.479	1.00	82.60	A
	ATOM	1030	CB	ILE	A	154	51.680	38.592	36.656	1.00	81.99	A
	ATOM	1031	CG2	ILE	A	154	51.889	38.898	38.134	0.00	82.34	A
	ATOM	1032	CG1	ILE	A	154	52.986	38.866	35.905	1.00	81.41	A
10	ATOM	1033	CD1	ILE	A	154	53.347	40.336	35.822	0.00	81.80	A
	ATOM	1034	C	ILE	A	154	49.976	36.834	37.285	1.00	83.80	A
	ATOM	1035	O	ILE	A	154	49.036	37.633	37.272	1.00	83.56	A
	ATOM	1036	N	ARG	A	155	49.956	35.697	37.982	1.00	85.60	A
	ATOM	1037	CA	ARG	A	155	48.807	35.284	38.783	1.00	86.76	A
15	ATOM	1038	CB	ARG	A	155	48.632	36.208	39.992	0.00	87.40	A
	ATOM	1039	CG	ARG	A	155	49.431	35.788	41.222	0.00	88.39	A
	ATOM	1040	CD	ARG	A	155	50.925	35.725	40.946	0.00	89.22	A
	ATOM	1041	NE	ARG	A	155	51.668	35.196	42.087	0.00	89.99	A
	ATOM	1042	CZ	ARG	A	155	51.561	33.949	42.535	0.00	90.38	A
20	ATOM	1043	NH1	ARG	A	155	50.740	33.095	41.937	0.00	90.63	A
	ATOM	1044	NH2	ARG	A	155	52.272	33.555	43.584	0.00	90.63	A
	ATOM	1045	C	ARG	A	155	47.543	35.286	37.933	1.00	87.04	A
	ATOM	1046	O	ARG	A	155	46.710	36.199	38.125	1.00	87.33	A
	ATOM	1047	OXT	ARG	A	155	47.413	34.380	37.075	1.00	86.76	A
25	ATOM	1048	CB	LEU	B	270	49.350	65.486	42.241	1.00	56.04	B
	ATOM	1049	CG	LEU	B	270	48.859	64.640	41.059	1.00	56.55	B
	ATOM	1050	CD1	LEU	B	270	47.337	64.629	41.020	1.00	55.59	B
	ATOM	1051	CD2	LEU	B	270	49.424	65.209	39.762	1.00	56.75	B
	ATOM	1052	C	LEU	B	270	49.537	63.882	44.208	1.00	54.79	B
30	ATOM	1053	O	LEU	B	270	50.136	63.918	45.287	1.00	55.23	B
	ATOM	1054	N	LEU	B	270	49.056	66.304	44.560	1.00	56.05	B
	ATOM	1055	CA	LEU	B	270	48.835	65.142	43.652	1.00	55.53	B
	ATOM	1056	N	LYS	B	271	49.463	62.779	43.462	1.00	52.96	B
	ATOM	1057	CA	LYS	B	271	50.053	61.495	43.865	1.00	49.38	B
35	ATOM	1058	CB	LYS	B	271	49.292	60.338	43.210	1.00	48.76	B
	ATOM	1059	CG	LYS	B	271	47.793	60.523	43.065	1.00	48.20	B
	ATOM	1060	CD	LYS	B	271	47.049	59.967	44.264	1.00	48.26	B
	ATOM	1061	CE	LYS	B	271	45.545	59.892	44.014	1.00	46.84	B
	ATOM	1062	NZ	LYS	B	271	45.188	59.152	42.766	1.00	47.61	B
40	ATOM	1063	C	LYS	B	271	51.521	61.364	43.462	1.00	47.55	B
	ATOM	1064	O	LYS	B	271	52.069	62.218	42.764	1.00	47.27	B
	ATOM	1065	N	ARG	B	272	52.138	60.263	43.883	1.00	45.44	B
	ATOM	1066	CA	ARG	B	272	53.529	59.981	43.558	1.00	42.97	B
	ATOM	1067	CB	ARG	B	272	54.444	60.845	44.404	1.00	42.52	B
45	ATOM	1068	CG	ARG	B	272	55.897	60.542	44.181	1.00	44.05	B
	ATOM	1069	CD	ARG	B	272	56.741	61.677	44.691	1.00	45.19	B
	ATOM	1070	NE	ARG	B	272	57.927	61.836	43.866	1.00	46.68	B
	ATOM	1071	CZ	ARG	B	272	58.416	63.009	43.491	1.00	47.36	B
	ATOM	1072	NH1	ARG	B	272	57.816	64.130	43.868	1.00	46.52	B
50	ATOM	1073	NH2	ARG	B	272	59.505	63.056	42.737	1.00	48.34	B
	ATOM	1074	C	ARG	B	272	53.911	58.517	43.753	1.00	41.43	B
	ATOM	1075	O	ARG	B	272	53.678	57.944	44.816	1.00	41.22	B
	ATOM	1076	N	ASP	B	273	54.495	57.911	42.724	1.00	39.99	B
	ATOM	1077	CA	ASP	B	273	54.914	56.517	42.821	1.00	37.49	B

ATOM	1078	CB	ASP	B	273	55.435	56.006	41.487	1.00	38.41	B
ATOM	1079	CG	ASP	B	273	55.631	54.508	41.482	1.00	40.70	B
ATOM	1080	OD1	ASP	B	273	56.269	53.969	42.423	1.00	39.39	B
ATOM	1081	OD2	ASP	B	273	55.143	53.874	40.525	1.00	43.85	B
ATOM	1082	C	ASP	B	273	56.040	56.474	43.829	1.00	35.40	B
ATOM	1083	O	ASP	B	273	57.218	56.453	43.463	1.00	33.99	B
ATOM	1084	N	LEU	B	274	55.671	56.460	45.101	1.00	33.28	B
ATOM	1085	CA	LEU	B	274	56.646	56.450	46.170	1.00	32.55	B
ATOM	1086	CB	LEU	B	274	55.937	56.322	47.514	1.00	32.85	B
ATOM	1087	CG	LEU	B	274	55.728	57.659	48.229	1.00	34.16	B
ATOM	1088	CD1	LEU	B	274	54.930	58.598	47.361	1.00	33.65	B
ATOM	1089	CD2	LEU	B	274	55.035	57.421	49.561	1.00	35.07	B
ATOM	1090	C	LEU	B	274	57.723	55.391	46.066	1.00	31.70	B
ATOM	1091	O	LEU	B	274	58.903	55.687	46.250	1.00	31.68	B
ATOM	1092	N	ILE	B	275	57.338	54.160	45.756	1.00	31.28	B
ATOM	1093	CA	ILE	B	275	58.338	53.115	45.687	1.00	30.61	B
ATOM	1094	CB	ILE	B	275	57.703	51.700	45.636	1.00	31.77	B
ATOM	1095	CG2	ILE	B	275	56.364	51.696	46.322	1.00	29.79	B
ATOM	1096	CG1	ILE	B	275	57.579	51.245	44.196	1.00	34.36	B
ATOM	1097	CD1	ILE	B	275	58.058	49.838	44.000	1.00	34.82	B
ATOM	1098	C	ILE	B	275	59.325	53.301	44.535	1.00	29.10	B
ATOM	1099	O	ILE	B	275	60.495	52.944	44.675	1.00	28.41	B
ATOM	1100	N	THR	B	276	58.893	53.846	43.398	1.00	28.07	B
ATOM	1101	CA	THR	B	276	59.875	54.056	42.336	1.00	29.79	B
ATOM	1102	CB	THR	B	276	59.259	54.160	40.906	1.00	29.82	B
ATOM	1103	OG1	THR	B	276	58.327	55.236	40.859	1.00	33.40	B
ATOM	1104	CG2	THR	B	276	58.569	52.869	40.507	1.00	31.42	B
ATOM	1105	C	THR	B	276	60.718	55.314	42.580	1.00	28.87	B
ATOM	1106	O	THR	B	276	61.885	55.341	42.222	1.00	29.74	B
ATOM	1107	N	SER	B	277	60.145	56.333	43.211	1.00	27.47	B
ATOM	1108	CA	SER	B	277	60.867	57.567	43.454	1.00	27.08	B
ATOM	1109	CB	SER	B	277	59.877	58.706	43.664	1.00	28.54	B
ATOM	1110	OG	SER	B	277	59.027	58.861	42.533	1.00	29.07	B
ATOM	1111	C	SER	B	277	61.843	57.511	44.622	1.00	28.04	B
ATOM	1112	O	SER	B	277	62.850	58.200	44.607	1.00	29.44	B
ATOM	1113	N	LEU	B	278	61.546	56.717	45.644	1.00	28.55	B
ATOM	1114	CA	LEU	B	278	62.443	56.606	46.786	1.00	28.04	B
ATOM	1115	CB	LEU	B	278	61.777	55.854	47.921	1.00	27.87	B
ATOM	1116	CG	LEU	B	278	61.098	56.650	49.043	1.00	29.93	B
ATOM	1117	CD1	LEU	B	278	62.130	57.593	49.658	1.00	30.19	B
ATOM	1118	CD2	LEU	B	278	59.898	57.407	48.526	1.00	28.70	B
ATOM	1119	C	LEU	B	278	63.697	55.857	46.401	1.00	29.78	B
ATOM	1120	O	LEU	B	278	63.728	55.140	45.398	1.00	30.41	B
ATOM	1121	N	PRO	B	279	64.771	56.039	47.171	1.00	30.02	B
ATOM	1122	CD	PRO	B	279	65.103	57.050	48.187	1.00	29.94	B
ATOM	1123	CA	PRO	B	279	65.948	55.281	46.764	1.00	30.32	B
ATOM	1124	CB	PRO	B	279	67.068	55.907	47.584	1.00	29.20	B
ATOM	1125	CG	PRO	B	279	66.371	56.499	48.763	1.00	31.41	B
ATOM	1126	C	PRO	B	279	65.690	53.813	47.094	1.00	32.64	B
ATOM	1127	O	PRO	B	279	64.946	53.494	48.026	1.00	32.21	B
ATOM	1128	N	PHE	B	280	66.291	52.927	46.308	1.00	34.93	B
ATOM	1129	CA	PHE	B	280	66.122	51.495	46.476	1.00	35.83	B
ATOM	1130	CB	PHE	B	280	67.177	50.745	45.671	1.00	35.18	B
ATOM	1131	CG	PHE	B	280	67.040	49.266	45.752	1.00	35.73	B

```
ATOM   1132  CD1 PHE B 280      65.871  48.644  45.307  1.00 35.82      B
ATOM   1133  CD2 PHE B 280      68.050  48.493  46.319  1.00 34.88      B
ATOM   1134  CE1 PHE B 280      65.703  47.266  45.430  1.00 37.94      B
ATOM   1135  CE2 PHE B 280      67.897  47.111  46.452  1.00 36.63      B
ATOM   1136  CZ  PHE B 280      66.717  46.489  46.006  1.00 36.74      B
ATOM   1137  C   PHE B 280      66.172  51.017  47.917  1.00 37.41      B
ATOM   1138  O   PHE B 280      65.263  50.331  48.371  1.00 39.64      B
ATOM   1139  N   GLU B 281      67.235  51.366  48.634  1.00 38.02      B
ATOM   1140  CA  GLU B 281      67.391  50.934  50.017  1.00 38.96      B
ATOM   1141  CB  GLU B 281      68.622  51.584  50.659  1.00 42.67      B
ATOM   1142  CG  GLU B 281      69.932  51.424  49.875  1.00 49.17      B
ATOM   1143  CD  GLU B 281      70.188  49.992  49.394  1.00 51.93      B
ATOM   1144  OE1 GLU B 281      69.840  49.030  50.127  1.00 51.55      B
ATOM   1145  OE2 GLU B 281      70.747  49.845  48.276  1.00 53.97      B
ATOM   1146  C   GLU B 281      66.169  51.251  50.859  1.00 38.70      B
ATOM   1147  O   GLU B 281      65.863  50.516  51.796  1.00 40.56      B
ATOM   1148  N   ILE B 282      65.472  52.338  50.531  1.00 36.39      B
ATOM   1149  CA  ILE B 282      64.289  52.728  51.291  1.00 33.47      B
ATOM   1150  CB  ILE B 282      64.019  54.250  51.194  1.00 33.48      B
ATOM   1151  CG2 ILE B 282      62.633  54.581  51.721  1.00 31.07      B
ATOM   1152  CG1 ILE B 282      65.091  55.007  51.974  1.00 33.33      B
ATOM   1153  CD1 ILE B 282      64.849  56.494  52.090  1.00 35.69      B
ATOM   1154  C   ILE B 282      63.030  51.984  50.891  1.00 32.60      B
ATOM   1155  O   ILE B 282      62.238  51.614  51.748  1.00 33.74      B
ATOM   1156  N   SER B 283      62.833  51.753  49.602  1.00 32.28      B
ATOM   1157  CA  SER B 283      61.632  51.052  49.180  1.00 31.76      B
ATOM   1158  CB  SER B 283      61.531  51.043  47.665  1.00 30.24      B
ATOM   1159  OG  SER B 283      60.948  52.260  47.227  1.00 30.65      B
ATOM   1160  C   SER B 283      61.554  49.642  49.732  1.00 32.64      B
ATOM   1161  O   SER B 283      60.460  49.145  50.033  1.00 31.74      B
ATOM   1162  N   LEU B 284      62.715  49.011  49.891  1.00 34.08      B
ATOM   1163  CA  LEU B 284      62.761  47.661  50.433  1.00 36.79      B
ATOM   1164  CB  LEU B 284      64.158  47.070  50.303  1.00 38.54      B
ATOM   1165  CG  LEU B 284      64.620  46.663  48.913  1.00 40.73      B
ATOM   1166  CD1 LEU B 284      65.953  45.935  49.085  1.00 41.39      B
ATOM   1167  CD2 LEU B 284      63.598  45.746  48.237  1.00 39.81      B
ATOM   1168  C   LEU B 284      62.331  47.606  51.903  1.00 37.57      B
ATOM   1169  O   LEU B 284      61.731  46.629  52.333  1.00 37.16      B
ATOM   1170  N   LYS B 285      62.654  48.636  52.679  1.00 37.42      B
ATOM   1171  CA  LYS B 285      62.258  48.638  54.071  1.00 37.32      B
ATOM   1172  CB  LYS B 285      62.706  49.927  54.757  1.00 37.90      B
ATOM   1173  CG  LYS B 285      64.221  50.101  54.711  1.00 41.29      B
ATOM   1174  CD  LYS B 285      64.714  51.417  55.305  1.00 43.06      B
ATOM   1175  CE  LYS B 285      64.504  51.487  56.811  1.00 44.78      B
ATOM   1176  NZ  LYS B 285      63.347  52.365  57.139  1.00 44.95      B
ATOM   1177  C   LYS B 285      60.754  48.531  54.078  1.00 36.58      B
ATOM   1178  O   LYS B 285      60.170  47.774  54.859  1.00 36.75      B
ATOM   1179  N   ILE B 286      60.137  49.268  53.163  1.00 34.81      B
ATOM   1180  CA  ILE B 286      58.687  49.286  53.038  1.00 34.65      B
ATOM   1181  CB  ILE B 286      58.233  50.340  51.988  1.00 35.18      B
ATOM   1182  CG2 ILE B 286      56.723  50.435  51.961  1.00 34.75      B
ATOM   1183  CG1 ILE B 286      58.778  51.721  52.361  1.00 36.78      B
ATOM   1184  CD1 ILE B 286      58.517  52.777  51.304  1.00 35.35      B
ATOM   1185  C   ILE B 286      58.141  47.909  52.646  1.00 34.49      B
```

```
ATOM   1186  O   ILE B 286      57.109  47.469  53.163  1.00 34.87      B
ATOM   1187  N   PHE B 287      58.825  47.232  51.726  1.00 32.88      B
ATOM   1188  CA  PHE B 287      58.373  45.915  51.300  1.00 30.31      B
ATOM   1189  CB  PHE B 287      59.086  45.501  50.002  1.00 26.38      B
ATOM   1190  CG  PHE B 287      58.530  46.184  48.785  1.00 23.19      B
ATOM   1191  CD1 PHE B 287      57.189  46.000  48.444  1.00 21.80      B
ATOM   1192  CD2 PHE B 287      59.300  47.078  48.043  1.00 20.28      B
ATOM   1193  CE1 PHE B 287      56.617  46.699  47.397  1.00 21.72      B
ATOM   1194  CE2 PHE B 287      58.740  47.788  46.985  1.00 21.62      B
ATOM   1195  CZ  PHE B 287      57.389  47.599  46.659  1.00 23.65      B
ATOM   1196  C   PHE B 287      58.566  44.899  52.419  1.00 31.61      B
ATOM   1197  O   PHE B 287      57.864  43.887  52.487  1.00 32.92      B
ATOM   1198  N   ASN B 288      59.498  45.191  53.320  1.00 32.92      B
ATOM   1199  CA  ASN B 288      59.747  44.316  54.460  1.00 34.33      B
ATOM   1200  CB  ASN B 288      61.117  44.574  55.067  1.00 34.27      B
ATOM   1201  CG  ASN B 288      62.228  43.993  54.243  1.00 35.15      B
ATOM   1202  OD1 ASN B 288      62.325  42.768  54.077  1.00 34.77      B
ATOM   1203  ND2 ASN B 288      63.086  44.865  53.717  1.00 37.02      B
ATOM   1204  C   ASN B 288      58.699  44.515  55.538  1.00 34.60      B
ATOM   1205  O   ASN B 288      58.700  43.801  56.537  1.00 35.55      B
ATOM   1206  N   TYR B 289      57.833  45.507  55.347  1.00 33.60      B
ATOM   1207  CA  TYR B 289      56.757  45.786  56.286  1.00 32.28      B
ATOM   1208  CB  TYR B 289      56.597  47.288  56.536  1.00 30.88      B
ATOM   1209  CG  TYR B 289      57.639  47.906  57.444  1.00 31.04      B
ATOM   1210  CD1 TYR B 289      57.824  47.445  58.743  1.00 29.76      B
ATOM   1211  CE1 TYR B 289      58.783  48.005  59.577  1.00 28.80      B
ATOM   1212  CD2 TYR B 289      58.441  48.954  57.001  1.00 30.42      B
ATOM   1213  CE2 TYR B 289      59.404  49.520  57.828  1.00 30.11      B
ATOM   1214  CZ  TYR B 289      59.572  49.036  59.117  1.00 29.29      B
ATOM   1215  OH  TYR B 289      60.550  49.565  59.927  1.00 27.49      B
ATOM   1216  C   TYR B 289      55.454  45.259  55.712  1.00 33.20      B
ATOM   1217  O   TYR B 289      54.381  45.681  56.131  1.00 34.61      B
ATOM   1218  N   LEU B 290      55.538  44.348  54.750  1.00 32.98      B
ATOM   1219  CA  LEU B 290      54.335  43.794  54.148  1.00 33.98      B
ATOM   1220  CB  LEU B 290      54.181  44.325  52.736  1.00 33.99      B
ATOM   1221  CG  LEU B 290      53.894  45.813  52.594  1.00 34.25      B
ATOM   1222  CD1 LEU B 290      53.690  46.102  51.123  1.00 32.35      B
ATOM   1223  CD2 LEU B 290      52.629  46.192  53.393  1.00 35.31      B
ATOM   1224  C   LEU B 290      54.340  42.284  54.112  1.00 35.59      B
ATOM   1225  O   LEU B 290      55.366  41.686  53.832  1.00 37.73      B
ATOM   1226  N   GLN B 291      53.200  41.660  54.390  1.00 36.68      B
ATOM   1227  CA  GLN B 291      53.126  40.198  54.364  1.00 37.99      B
ATOM   1228  CB  GLN B 291      51.808  39.715  54.956  1.00 39.90      B
ATOM   1229  CG  GLN B 291      51.514  40.243  56.338  1.00 42.72      B
ATOM   1230  CD  GLN B 291      50.510  39.378  57.067  1.00 45.38      B
ATOM   1231  OE1 GLN B 291      49.376  39.196  56.609  1.00 45.17      B
ATOM   1232  NE2 GLN B 291      50.925  38.824  58.209  1.00 48.06      B
ATOM   1233  C   GLN B 291      53.254  39.696  52.937  1.00 37.97      B
ATOM   1234  O   GLN B 291      52.727  40.304  52.005  1.00 37.21      B
ATOM   1235  N   PHE B 292      53.924  38.566  52.769  1.00 39.53      B
ATOM   1236  CA  PHE B 292      54.154  38.038  51.430  1.00 42.10      B
ATOM   1237  CB  PHE B 292      54.592  36.565  51.510  1.00 43.75      B
ATOM   1238  CG  PHE B 292      53.463  35.605  51.727  1.00 44.90      B
ATOM   1239  CD1 PHE B 292      52.799  35.038  50.641  1.00 43.90      B
```

ATOM	1240	CD2	PHE	B	292	53.050	35.280	53.014	1.00	45.10	B
ATOM	1241	CE1	PHE	B	292	51.742	34.161	50.831	1.00	43.67	B
ATOM	1242	CE2	PHE	B	292	51.992	34.403	53.217	1.00	44.65	B
ATOM	1243	CZ	PHE	B	292	51.336	33.842	52.121	1.00	44.41	B
ATOM	1244	C	PHE	B	292	52.990	38.217	50.441	1.00	42.01	B
ATOM	1245	O	PHE	B	292	53.214	38.553	49.280	1.00	43.29	B
ATOM	1246	N	GLU	B	293	51.753	38.018	50.884	1.00	41.02	B
ATOM	1247	CA	GLU	B	293	50.605	38.176	49.985	1.00	40.82	B
ATOM	1248	CB	GLU	B	293	49.289	38.028	50.769	1.00	41.39	B
ATOM	1249	CG	GLU	B	293	49.056	36.617	51.350	1.00	42.89	B
ATOM	1250	CD	GLU	B	293	49.451	36.480	52.818	1.00	43.53	B
ATOM	1251	OE1	GLU	B	293	50.507	37.006	53.222	1.00	44.09	B
ATOM	1252	OE2	GLU	B	293	48.704	35.825	53.572	1.00	45.55	B
ATOM	1253	C	GLU	B	293	50.641	39.524	49.258	1.00	40.05	B
ATOM	1254	O	GLU	B	293	50.375	39.603	48.056	1.00	38.85	B
ATOM	1255	N	ASP	B	294	50.991	40.573	50.000	1.00	40.23	B
ATOM	1256	CA	ASP	B	294	51.074	41.923	49.450	1.00	40.33	B
ATOM	1257	CB	ASP	B	294	51.198	42.958	50.579	1.00	41.12	B
ATOM	1258	CG	ASP	B	294	49.949	43.030	51.464	1.00	42.16	B
ATOM	1259	OD1	ASP	B	294	48.815	42.987	50.925	1.00	43.30	B
ATOM	1260	OD2	ASP	B	294	50.099	43.150	52.699	1.00	41.57	B
ATOM	1261	C	ASP	B	294	52.259	42.074	48.490	1.00	38.83	B
ATOM	1262	O	ASP	B	294	52.151	42.714	47.446	1.00	37.73	B
ATOM	1263	N	ILE	B	295	53.390	41.477	48.840	1.00	37.53	B
ATOM	1264	CA	ILE	B	295	54.561	41.573	47.994	1.00	36.43	B
ATOM	1265	CB	ILE	B	295	55.751	40.853	48.638	1.00	35.75	B
ATOM	1266	CG2	ILE	B	295	56.926	40.801	47.660	1.00	35.40	B
ATOM	1267	CG1	ILE	B	295	56.107	41.574	49.950	1.00	36.24	B
ATOM	1268	CD1	ILE	B	295	57.303	41.033	50.709	1.00	36.08	B
ATOM	1269	C	ILE	B	295	54.257	40.987	46.623	1.00	36.37	B
ATOM	1270	O	ILE	B	295	54.707	41.504	45.593	1.00	36.01	B
ATOM	1271	N	ILE	B	296	53.470	39.919	46.616	1.00	36.36	B
ATOM	1272	CA	ILE	B	296	53.094	39.262	45.375	1.00	36.96	B
ATOM	1273	CB	ILE	B	296	52.329	37.967	45.665	1.00	37.13	B
ATOM	1274	CG2	ILE	B	296	51.771	37.366	44.389	1.00	37.11	B
ATOM	1275	CG1	ILE	B	296	53.276	36.961	46.288	1.00	36.41	B
ATOM	1276	CD1	ILE	B	296	52.601	35.679	46.620	1.00	38.88	B
ATOM	1277	C	ILE	B	296	52.256	40.159	44.473	1.00	36.89	B
ATOM	1278	O	ILE	B	296	52.554	40.297	43.293	1.00	37.07	B
ATOM	1279	N	ASN	B	297	51.208	40.769	45.008	1.00	37.95	B
ATOM	1280	CA	ASN	B	297	50.385	41.649	44.186	1.00	38.86	B
ATOM	1281	CB	ASN	B	297	49.240	42.246	44.980	1.00	41.69	B
ATOM	1282	CG	ASN	B	297	48.368	41.213	45.583	1.00	43.05	B
ATOM	1283	OD1	ASN	B	297	47.914	40.293	44.897	1.00	44.19	B
ATOM	1284	ND2	ASN	B	297	48.114	41.345	46.880	1.00	43.88	B
ATOM	1285	C	ASN	B	297	51.207	42.810	43.705	1.00	37.72	B
ATOM	1286	O	ASN	B	297	50.953	43.360	42.632	1.00	36.87	B
ATOM	1287	N	SER	B	298	52.167	43.207	44.531	1.00	36.60	B
ATOM	1288	CA	SER	B	298	53.006	44.339	44.194	1.00	35.31	B
ATOM	1289	CB	SER	B	298	53.926	44.673	45.366	1.00	32.10	B
ATOM	1290	OG	SER	B	298	53.156	45.195	46.435	1.00	29.27	B
ATOM	1291	C	SER	B	298	53.784	44.022	42.939	1.00	35.81	B
ATOM	1292	O	SER	B	298	54.037	44.901	42.111	1.00	35.32	B
ATOM	1293	N	LEU	B	299	54.136	42.750	42.793	1.00	36.25	B

```
ATOM   1294  CA  LEU B 299      54.871  42.291  41.625  1.00 36.42      B
ATOM   1295  CB  LEU B 299      55.218  40.814  41.771  1.00 35.83      B
ATOM   1296  CG  LEU B 299      56.431  40.528  42.654  1.00 36.52      B
ATOM   1297  CD1 LEU B 299      56.674  39.028  42.727  1.00 37.64      B
ATOM   1298  CD2 LEU B 299      57.655  41.224  42.065  1.00 35.78      B
ATOM   1299  C   LEU B 299      54.082  42.509  40.343  1.00 36.00      B
ATOM   1300  O   LEU B 299      54.660  42.539  39.256  1.00 36.92      B
ATOM   1301  N   GLY B 300      52.769  42.678  40.474  1.00 35.04      B
ATOM   1302  CA  GLY B 300      51.940  42.890  39.303  1.00 35.67      B
ATOM   1303  C   GLY B 300      51.417  44.305  39.186  1.00 35.69      B
ATOM   1304  O   GLY B 300      50.538  44.602  38.379  1.00 35.37      B
ATOM   1305  N   VAL B 301      51.958  45.194  39.998  1.00 36.32      B
ATOM   1306  CA  VAL B 301      51.523  46.569  39.969  1.00 36.62      B
ATOM   1307  CB  VAL B 301      51.953  47.291  41.247  1.00 37.56      B
ATOM   1308  CG1 VAL B 301      51.752  48.789  41.087  1.00 37.50      B
ATOM   1309  CG2 VAL B 301      51.133  46.752  42.436  1.00 35.20      B
ATOM   1310  C   VAL B 301      52.071  47.288  38.751  1.00 36.72      B
ATOM   1311  O   VAL B 301      51.321  47.910  38.017  1.00 37.30      B
ATOM   1312  N   SER B 302      53.378  47.201  38.534  1.00 37.60      B
ATOM   1313  CA  SER B 302      54.005  47.844  37.382  1.00 37.90      B
ATOM   1314  CB  SER B 302      54.317  49.311  37.684  1.00 37.39      B
ATOM   1315  OG  SER B 302      55.530  49.417  38.419  1.00 36.20      B
ATOM   1316  C   SER B 302      55.316  47.129  37.067  1.00 39.64      B
ATOM   1317  O   SER B 302      55.867  46.392  37.901  1.00 38.64      B
ATOM   1318  N   GLN B 303      55.821  47.371  35.861  1.00 40.39      B
ATOM   1319  CA  GLN B 303      57.087  46.781  35.428  1.00 41.46      B
ATOM   1320  CB  GLN B 303      57.436  47.239  34.013  1.00 41.20      B
ATOM   1321  CG  GLN B 303      56.696  46.481  32.950  1.00 43.64      B
ATOM   1322  CD  GLN B 303      57.199  45.068  32.815  1.00 44.54      B
ATOM   1323  OE1 GLN B 303      57.771  44.517  33.751  1.00 46.50      B
ATOM   1324  NE2 GLN B 303      56.986  44.466  31.650  1.00 44.23      B
ATOM   1325  C   GLN B 303      58.241  47.140  36.360  1.00 41.74      B
ATOM   1326  O   GLN B 303      59.163  46.345  36.561  1.00 41.80      B
ATOM   1327  N   ASN B 304      58.194  48.338  36.928  1.00 42.15      B
ATOM   1328  CA  ASN B 304      59.251  48.758  37.826  1.00 41.69      B
ATOM   1329  CB  ASN B 304      59.237  50.263  38.014  1.00 43.58      B
ATOM   1330  CG  ASN B 304      60.623  50.861  37.924  1.00 45.74      B
ATOM   1331  OD1 ASN B 304      61.599  50.302  38.459  1.00 46.54      B
ATOM   1332  ND2 ASN B 304      60.728  52.009  37.240  1.00 47.34      B
ATOM   1333  C   ASN B 304      59.130  48.100  39.174  1.00 41.16      B
ATOM   1334  O   ASN B 304      60.126  47.650  39.739  1.00 40.69      B
ATOM   1335  N   TRP B 305      57.910  48.060  39.700  1.00 40.22      B
ATOM   1336  CA  TRP B 305      57.687  47.439  40.992  1.00 39.44      B
ATOM   1337  CB  TRP B 305      56.201  47.464  41.357  1.00 40.05      B
ATOM   1338  CG  TRP B 305      55.742  48.762  41.945  1.00 41.46      B
ATOM   1339  CD2 TRP B 305      54.933  48.939  43.120  1.00 42.85      B
ATOM   1340  CE2 TRP B 305      54.724  50.324  43.277  1.00 43.18      B
ATOM   1341  CE3 TRP B 305      54.363  48.060  44.054  1.00 43.70      B
ATOM   1342  CD1 TRP B 305      55.983  50.007  41.456  1.00 41.95      B
ATOM   1343  NE1 TRP B 305      55.375  50.953  42.248  1.00 43.45      B
ATOM   1344  CZ2 TRP B 305      53.966  50.858  44.336  1.00 43.29      B
ATOM   1345  CZ3 TRP B 305      53.608  48.591  45.108  1.00 43.59      B
ATOM   1346  CH2 TRP B 305      53.419  49.976  45.237  1.00 43.13      B
ATOM   1347  C   TRP B 305      58.186  46.007  40.930  1.00 39.39      B
```

```
ATOM   1348  O   TRP B 305      58.909  45.556  41.818  1.00 40.05      B
ATOM   1349  N   ASN B 306      57.808  45.300  39.868  1.00 38.31      B
ATOM   1350  CA  ASN B 306      58.213  43.915  39.699  1.00 36.89      B
ATOM   1351  CB  ASN B 306      57.558  43.318  38.449  1.00 39.69      B
ATOM   1352  CG  ASN B 306      57.874  41.836  38.265  1.00 41.87      B
ATOM   1353  OD1 ASN B 306      58.898  41.465  37.690  1.00 42.36      B
ATOM   1354  ND2 ASN B 306      56.989  40.983  38.763  1.00 44.37      B
ATOM   1355  C   ASN B 306      59.730  43.817  39.608  1.00 35.41      B
ATOM   1356  O   ASN B 306      60.333  42.902  40.170  1.00 35.33      B
ATOM   1357  N   LYS B 307      60.353  44.765  38.917  1.00 34.02      B
ATOM   1358  CA  LYS B 307      61.804  44.750  38.786  1.00 34.18      B
ATOM   1359  CB  LYS B 307      62.245  45.720  37.686  1.00 34.16      B
ATOM   1360  CG  LYS B 307      63.753  45.889  37.572  1.00 34.46      B
ATOM   1361  CD  LYS B 307      64.121  46.934  36.524  1.00 36.66      B
ATOM   1362  CE  LYS B 307      63.783  46.479  35.089  1.00 39.17      B
ATOM   1363  NZ  LYS B 307      62.308  46.327  34.816  1.00 41.27      B
ATOM   1364  C   LYS B 307      62.491  45.096  40.110  1.00 34.15      B
ATOM   1365  O   LYS B 307      63.484  44.476  40.486  1.00 35.79      B
ATOM   1366  N   ILE B 308      61.967  46.089  40.814  1.00 33.56      B
ATOM   1367  CA  ILE B 308      62.539  46.483  42.090  1.00 32.11      B
ATOM   1368  CB  ILE B 308      61.790  47.706  42.670  1.00 31.25      B
ATOM   1369  CG2 ILE B 308      62.235  47.954  44.118  1.00 29.28      B
ATOM   1370  CG1 ILE B 308      62.010  48.918  41.746  1.00 30.74      B
ATOM   1371  CD1 ILE B 308      61.163  50.148  42.057  1.00 30.81      B
ATOM   1372  C   ILE B 308      62.455  45.330  43.083  1.00 32.53      B
ATOM   1373  O   ILE B 308      63.432  44.996  43.741  1.00 33.24      B
ATOM   1374  N   ILE B 309      61.288  44.706  43.174  1.00 32.71      B
ATOM   1375  CA  ILE B 309      61.094  43.616  44.120  1.00 32.29      B
ATOM   1376  CB  ILE B 309      59.605  43.255  44.224  1.00 31.48      B
ATOM   1377  CG2 ILE B 309      59.436  41.944  44.993  1.00 28.42      B
ATOM   1378  CG1 ILE B 309      58.860  44.419  44.894  1.00 29.43      B
ATOM   1379  CD1 ILE B 309      57.377  44.244  45.030  1.00 29.32      B
ATOM   1380  C   ILE B 309      61.881  42.360  43.801  1.00 32.95      B
ATOM   1381  O   ILE B 309      62.297  41.616  44.705  1.00 33.10      B
ATOM   1382  N   ARG B 310      62.088  42.120  42.515  1.00 32.48      B
ATOM   1383  CA  ARG B 310      62.807  40.929  42.113  1.00 31.41      B
ATOM   1384  CB  ARG B 310      62.401  40.562  40.701  1.00 30.53      B
ATOM   1385  CG  ARG B 310      61.047  39.954  40.749  1.00 32.30      B
ATOM   1386  CD  ARG B 310      60.974  38.823  39.812  1.00 33.94      B
ATOM   1387  NE  ARG B 310      60.659  39.310  38.485  1.00 36.53      B
ATOM   1388  CZ  ARG B 310      60.989  38.682  37.369  1.00 37.75      B
ATOM   1389  NH1 ARG B 310      61.656  37.535  37.428  1.00 36.97      B
ATOM   1390  NH2 ARG B 310      60.649  39.205  36.200  1.00 38.45      B
ATOM   1391  C   ARG B 310      64.302  41.065  42.259  1.00 30.16      B
ATOM   1392  O   ARG B 310      65.059  40.091  42.152  1.00 28.61      B
ATOM   1393  N   LYS B 311      64.717  42.283  42.552  1.00 29.95      B
ATOM   1394  CA  LYS B 311      66.122  42.542  42.727  1.00 31.78      B
ATOM   1395  CB  LYS B 311      66.419  44.014  42.471  1.00 30.98      B
ATOM   1396  CG  LYS B 311      67.876  44.355  42.676  1.00 34.65      B
ATOM   1397  CD  LYS B 311      68.141  45.839  42.539  0.00 34.39      B
ATOM   1398  CE  LYS B 311      68.033  46.305  41.095  0.00 35.04      B
ATOM   1399  NZ  LYS B 311      66.665  46.176  40.520  0.00 35.23      B
ATOM   1400  C   LYS B 311      66.589  42.154  44.127  1.00 31.89      B
ATOM   1401  O   LYS B 311      67.761  41.815  44.325  1.00 31.11      B
```

```
ATOM   1402  N   SER B 312      65.666  42.181  45.088  1.00 32.44      B
ATOM   1403  CA  SER B 312      65.997  41.868  46.479  1.00 34.40      B
ATOM   1404  CB  SER B 312      64.998  42.541  47.433  1.00 35.97      B
ATOM   1405  OG  SER B 312      65.318  42.268  48.793  1.00 37.24      B
ATOM   1406  C   SER B 312      66.068  40.389  46.825  1.00 33.58      B
ATOM   1407  O   SER B 312      65.154  39.629  46.532  1.00 35.14      B
ATOM   1408  N   THR B 313      67.160  39.990  47.460  1.00 32.17      B
ATOM   1409  CA  THR B 313      67.314  38.613  47.867  1.00 32.11      B
ATOM   1410  CB  THR B 313      68.760  38.142  47.682  1.00 34.02      B
ATOM   1411  OG1 THR B 313      68.921  37.648  46.346  1.00 35.15      B
ATOM   1412  CG2 THR B 313      69.114  37.055  48.685  1.00 33.55      B
ATOM   1413  C   THR B 313      66.913  38.532  49.329  1.00 30.50      B
ATOM   1414  O   THR B 313      66.318  37.553  49.764  1.00 31.15      B
ATOM   1415  N   SER B 314      67.219  39.583  50.078  1.00 29.28      B
ATOM   1416  CA  SER B 314      66.881  39.648  51.493  1.00 28.64      B
ATOM   1417  CB  SER B 314      67.307  40.990  52.076  1.00 28.48      B
ATOM   1418  OG  SER B 314      68.696  40.979  52.349  1.00 33.47      B
ATOM   1419  C   SER B 314      65.397  39.479  51.710  1.00 27.68      B
ATOM   1420  O   SER B 314      64.966  38.738  52.592  1.00 28.00      B
ATOM   1421  N   LEU B 315      64.629  40.182  50.890  1.00 25.95      B
ATOM   1422  CA  LEU B 315      63.190  40.158  50.967  1.00 24.83      B
ATOM   1423  CB  LEU B 315      62.614  40.721  49.676  1.00 22.38      B
ATOM   1424  CG  LEU B 315      61.151  41.129  49.740  1.00 21.41      B
ATOM   1425  CD1 LEU B 315      61.006  42.400  50.604  1.00 20.01      B
ATOM   1426  CD2 LEU B 315      60.662  41.376  48.345  1.00 19.89      B
ATOM   1427  C   LEU B 315      62.675  38.745  51.206  1.00 26.71      B
ATOM   1428  O   LEU B 315      61.894  38.494  52.141  1.00 27.54      B
ATOM   1429  N   TRP B 316      63.110  37.813  50.369  1.00 26.88      B
ATOM   1430  CA  TRP B 316      62.665  36.439  50.534  1.00 27.42      B
ATOM   1431  CB  TRP B 316      62.776  35.691  49.204  1.00 27.04      B
ATOM   1432  CG  TRP B 316      62.021  36.416  48.176  1.00 25.52      B
ATOM   1433  CD2 TRP B 316      60.600  36.519  48.088  1.00 25.34      B
ATOM   1434  CE2 TRP B 316      60.313  37.456  47.071  1.00 24.36      B
ATOM   1435  CE3 TRP B 316      59.540  35.920  48.778  1.00 26.16      B
ATOM   1436  CD1 TRP B 316      62.526  37.262  47.232  1.00 25.54      B
ATOM   1437  NE1 TRP B 316      61.507  37.892  46.566  1.00 23.85      B
ATOM   1438  CZ2 TRP B 316      59.003  37.808  46.728  1.00 23.50      B
ATOM   1439  CZ3 TRP B 316      58.236  36.272  48.438  1.00 24.82      B
ATOM   1440  CH2 TRP B 316      57.981  37.209  47.421  1.00 24.99      B
ATOM   1441  C   TRP B 316      63.402  35.720  51.656  1.00 27.65      B
ATOM   1442  O   TRP B 316      62.786  34.989  52.446  1.00 27.76      B
ATOM   1443  N   LYS B 317      64.709  35.934  51.744  1.00 27.10      B
ATOM   1444  CA  LYS B 317      65.455  35.304  52.817  1.00 28.92      B
ATOM   1445  CB  LYS B 317      66.907  35.788  52.830  1.00 30.51      B
ATOM   1446  CG  LYS B 317      67.768  35.175  53.935  1.00 32.68      B
ATOM   1447  CD  LYS B 317      69.209  35.655  53.820  1.00 35.89      B
ATOM   1448  CE  LYS B 317      69.849  35.839  55.186  1.00 37.32      B
ATOM   1449  NZ  LYS B 317      69.169  36.927  55.978  1.00 39.48      B
ATOM   1450  C   LYS B 317      64.764  35.597  54.164  1.00 29.21      B
ATOM   1451  O   LYS B 317      64.560  34.682  54.975  1.00 28.72      B
ATOM   1452  N   LYS B 318      64.373  36.851  54.394  1.00 27.41      B
ATOM   1453  CA  LYS B 318      63.698  37.182  55.640  1.00 27.23      B
ATOM   1454  CB  LYS B 318      63.287  38.657  55.685  1.00 28.22      B
ATOM   1455  CG  LYS B 318      64.448  39.580  55.982  1.00 29.33      B
```

```
ATOM   1456  CD  LYS B 318      64.011  40.989  56.263  1.00 29.29      B
ATOM   1457  CE  LYS B 318      65.211  41.805  56.726  1.00 31.20      B
ATOM   1458  NZ  LYS B 318      66.332  41.748  55.749  1.00 29.62      B
ATOM   1459  C   LYS B 318      62.475  36.318  55.846  1.00 28.19      B
ATOM   1460  O   LYS B 318      62.325  35.651  56.881  1.00 29.19      B
ATOM   1461  N   LEU B 319      61.598  36.346  54.847  1.00 28.31      B
ATOM   1462  CA  LEU B 319      60.353  35.576  54.851  1.00 26.08      B
ATOM   1463  CB  LEU B 319      59.644  35.756  53.499  1.00 24.60      B
ATOM   1464  CG  LEU B 319      58.949  37.106  53.299  1.00 23.31      B
ATOM   1465  CD1 LEU B 319      58.929  37.501  51.828  1.00 25.42      B
ATOM   1466  CD2 LEU B 319      57.550  37.030  53.849  1.00 20.66      B
ATOM   1467  C   LEU B 319      60.661  34.104  55.115  1.00 24.68      B
ATOM   1468  O   LEU B 319      60.126  33.511  56.051  1.00 24.33      B
ATOM   1469  N   LEU B 320      61.521  33.515  54.292  1.00 24.37      B
ATOM   1470  CA  LEU B 320      61.887  32.119  54.496  1.00 24.33      B
ATOM   1471  CB  LEU B 320      63.119  31.777  53.678  1.00 20.97      B
ATOM   1472  CG  LEU B 320      62.711  31.425  52.272  1.00 20.93      B
ATOM   1473  CD1 LEU B 320      63.945  31.333  51.431  1.00 21.63      B
ATOM   1474  CD2 LEU B 320      61.936  30.117  52.276  1.00 17.66      B
ATOM   1475  C   LEU B 320      62.166  31.800  55.967  1.00 24.55      B
ATOM   1476  O   LEU B 320      61.744  30.769  56.491  1.00 25.31      B
ATOM   1477  N   ILE B 321      62.883  32.706  56.615  1.00 24.47      B
ATOM   1478  CA  ILE B 321      63.253  32.579  58.009  1.00 23.96      B
ATOM   1479  CB  ILE B 321      64.450  33.531  58.315  1.00 25.52      B
ATOM   1480  CG2 ILE B 321      64.759  33.556  59.806  1.00 25.19      B
ATOM   1481  CG1 ILE B 321      65.671  33.094  57.498  1.00 23.92      B
ATOM   1482  CD1 ILE B 321      66.951  33.873  57.782  1.00 24.41      B
ATOM   1483  C   ILE B 321      62.065  32.882  58.928  1.00 23.22      B
ATOM   1484  O   ILE B 321      61.902  32.240  59.952  1.00 24.18      B
ATOM   1485  N   SER B 322      61.239  33.853  58.563  1.00 23.04      B
ATOM   1486  CA  SER B 322      60.079  34.200  59.370  1.00 23.65      B
ATOM   1487  CB  SER B 322      59.248  35.266  58.670  1.00 21.62      B
ATOM   1488  OG  SER B 322      60.030  36.403  58.387  1.00 24.32      B
ATOM   1489  C   SER B 322      59.203  32.990  59.581  1.00 24.95      B
ATOM   1490  O   SER B 322      58.789  32.691  60.696  1.00 28.00      B
ATOM   1491  N   GLU B 323      58.926  32.302  58.485  1.00 25.30      B
ATOM   1492  CA  GLU B 323      58.066  31.135  58.486  1.00 25.97      B
ATOM   1493  CB  GLU B 323      57.480  30.974  57.091  1.00 26.35      B
ATOM   1494  CG  GLU B 323      56.792  32.239  56.646  1.00 27.43      B
ATOM   1495  CD  GLU B 323      55.441  32.431  57.307  1.00 27.80      B
ATOM   1496  OE1 GLU B 323      55.239  31.878  58.409  1.00 25.90      B
ATOM   1497  OE2 GLU B 323      54.590  33.142  56.718  1.00 28.13      B
ATOM   1498  C   GLU B 323      58.745  29.855  58.917  1.00 25.13      B
ATOM   1499  O   GLU B 323      58.123  28.792  58.931  1.00 25.20      B
ATOM   1500  N   ASN B 324      60.019  29.966  59.276  1.00 24.08      B
ATOM   1501  CA  ASN B 324      60.808  28.816  59.708  1.00 24.96      B
ATOM   1502  CB  ASN B 324      60.203  28.185  60.974  1.00 26.02      B
ATOM   1503  CG  ASN B 324      60.051  29.187  62.108  1.00 28.82      B
ATOM   1504  OD1 ASN B 324      61.030  29.766  62.605  1.00 29.61      B
ATOM   1505  ND2 ASN B 324      58.813  29.402  62.518  1.00 29.76      B
ATOM   1506  C   ASN B 324      60.906  27.776  58.588  1.00 24.92      B
ATOM   1507  O   ASN B 324      60.642  26.596  58.786  1.00 23.18      B
ATOM   1508  N   PHE B 325      61.269  28.226  57.395  1.00 25.71      B
ATOM   1509  CA  PHE B 325      61.406  27.304  56.287  1.00 25.91      B
```

```
ATOM   1510  CB  PHE B 325      60.839  27.913  55.008  1.00 24.25      B
ATOM   1511  CG  PHE B 325      59.334  27.935  54.987  1.00 23.73      B
ATOM   1512  CD1 PHE B 325      58.644  28.984  54.394  1.00 23.04      B
ATOM   1513  CD2 PHE B 325      58.604  26.925  55.616  1.00 20.21      B
ATOM   1514  CE1 PHE B 325      57.259  29.025  54.437  1.00 20.96      B
ATOM   1515  CE2 PHE B 325      57.227  26.964  55.658  1.00 18.74      B
ATOM   1516  CZ  PHE B 325      56.555  28.015  55.073  1.00 19.51      B
ATOM   1517  C   PHE B 325      62.861  26.972  56.156  1.00 26.92      B
ATOM   1518  O   PHE B 325      63.232  26.019  55.478  1.00 28.62      B
ATOM   1519  N   VAL B 326      63.683  27.766  56.833  1.00 27.50      B
ATOM   1520  CA  VAL B 326      65.127  27.577  56.849  1.00 27.18      B
ATOM   1521  CB  VAL B 326      65.773  28.060  55.532  1.00 25.75      B
ATOM   1522  CG1 VAL B 326      66.019  29.553  55.587  1.00 23.02      B
ATOM   1523  CG2 VAL B 326      67.061  27.316  55.288  1.00 26.04      B
ATOM   1524  C   VAL B 326      65.685  28.408  57.993  1.00 28.22      B
ATOM   1525  O   VAL B 326      64.998  29.274  58.533  1.00 28.23      B
ATOM   1526  N   SER B 327      66.932  28.154  58.361  1.00 29.87      B
ATOM   1527  CA  SER B 327      67.547  28.926  59.427  1.00 32.04      B
ATOM   1528  CB  SER B 327      67.867  28.053  60.643  1.00 32.92      B
ATOM   1529  OG  SER B 327      69.012  27.244  60.404  1.00 35.60      B
ATOM   1530  C   SER B 327      68.837  29.511  58.905  1.00 33.44      B
ATOM   1531  O   SER B 327      69.404  29.024  57.925  1.00 35.13      B
ATOM   1532  N   PRO B 328      69.328  30.561  59.568  1.00 34.95      B
ATOM   1533  CD  PRO B 328      68.703  31.277  60.698  1.00 34.72      B
ATOM   1534  CA  PRO B 328      70.570  31.208  59.161  1.00 35.43      B
ATOM   1535  CB  PRO B 328      70.906  32.056  60.372  1.00 34.44      B
ATOM   1536  CG  PRO B 328      69.541  32.530  60.792  1.00 34.00      B
ATOM   1537  C   PRO B 328      71.674  30.211  58.789  1.00 37.33      B
ATOM   1538  O   PRO B 328      72.413  30.428  57.820  1.00 38.07      B
ATOM   1539  N   LYS B 329      71.779  29.106  59.524  1.00 38.13      B
ATOM   1540  CA  LYS B 329      72.830  28.126  59.222  1.00 39.44      B
ATOM   1541  CB  LYS B 329      73.088  27.201  60.423  1.00 41.96      B
ATOM   1542  CG  LYS B 329      73.334  27.911  61.736  1.00 44.54      B
ATOM   1543  CD  LYS B 329      74.564  28.801  61.693  1.00 46.08      B
ATOM   1544  CE  LYS B 329      74.745  29.475  63.047  1.00 47.88      B
ATOM   1545  NZ  LYS B 329      73.510  30.241  63.384  1.00 48.71      B
ATOM   1546  C   LYS B 329      72.539  27.255  58.005  1.00 38.23      B
ATOM   1547  O   LYS B 329      73.444  26.922  57.230  1.00 37.43      B
ATOM   1548  N   GLY B 330      71.279  26.863  57.858  1.00 36.83      B
ATOM   1549  CA  GLY B 330      70.904  26.026  56.733  1.00 34.91      B
ATOM   1550  C   GLY B 330      70.671  26.809  55.458  1.00 33.34      B
ATOM   1551  O   GLY B 330      70.432  26.217  54.402  1.00 31.96      B
ATOM   1552  N   PHE B 331      70.742  28.136  55.554  1.00 32.27      B
ATOM   1553  CA  PHE B 331      70.517  28.977  54.388  1.00 32.81      B
ATOM   1554  CB  PHE B 331      70.778  30.454  54.688  1.00 32.71      B
ATOM   1555  CG  PHE B 331      70.365  31.374  53.561  1.00 35.02      B
ATOM   1556  CD1 PHE B 331      69.013  31.631  53.319  1.00 34.88      B
ATOM   1557  CD2 PHE B 331      71.323  31.971  52.727  1.00 36.79      B
ATOM   1558  CE1 PHE B 331      68.609  32.466  52.274  1.00 35.03      B
ATOM   1559  CE2 PHE B 331      70.933  32.816  51.670  1.00 36.82      B
ATOM   1560  CZ  PHE B 331      69.568  33.061  51.446  1.00 36.85      B
ATOM   1561  C   PHE B 331      71.333  28.600  53.164  1.00 32.72      B
ATOM   1562  O   PHE B 331      70.779  28.197  52.143  1.00 32.53      B
ATOM   1563  N   ASN B 332      72.650  28.725  53.261  1.00 33.63      B
```

```
ATOM   1564  CA  ASN B 332      73.495  28.430  52.116  1.00 34.96      B
ATOM   1565  CB  ASN B 332      74.956  28.510  52.503  1.00 35.07      B
ATOM   1566  CG  ASN B 332      75.386  29.925  52.769  1.00 36.45      B
ATOM   1567  OD1 ASN B 332      74.860  30.864  52.165  1.00 36.09      B
ATOM   1568  ND2 ASN B 332      76.352  30.096  53.666  1.00 37.34      B
ATOM   1569  C   ASN B 332      73.204  27.105  51.457  1.00 35.37      B
ATOM   1570  O   ASN B 332      73.006  27.034  50.240  1.00 34.82      B
ATOM   1571  N   SER B 333      73.174  26.050  52.253  1.00 36.35      B
ATOM   1572  CA  SER B 333      72.897  24.749  51.696  1.00 38.23      B
ATOM   1573  CB  SER B 333      72.767  23.724  52.804  1.00 37.83      B
ATOM   1574  OG  SER B 333      72.509  22.458  52.236  1.00 43.08      B
ATOM   1575  C   SER B 333      71.615  24.785  50.867  1.00 38.81      B
ATOM   1576  O   SER B 333      71.522  24.144  49.814  1.00 39.26      B
ATOM   1577  N   LEU B 334      70.629  25.533  51.357  1.00 38.86      B
ATOM   1578  CA  LEU B 334      69.338  25.688  50.685  1.00 37.16      B
ATOM   1579  CB  LEU B 334      68.446  26.645  51.486  1.00 34.21      B
ATOM   1580  CG  LEU B 334      67.149  27.126  50.830  1.00 33.30      B
ATOM   1581  CD1 LEU B 334      66.189  25.957  50.642  1.00 29.33      B
ATOM   1582  CD2 LEU B 334      66.528  28.209  51.688  1.00 31.65      B
ATOM   1583  C   LEU B 334      69.574  26.251  49.291  1.00 37.44      B
ATOM   1584  O   LEU B 334      69.105  25.700  48.293  1.00 36.40      B
ATOM   1585  N   ASN B 335      70.306  27.361  49.248  1.00 38.10      B
ATOM   1586  CA  ASN B 335      70.647  28.032  48.001  1.00 38.02      B
ATOM   1587  CB  ASN B 335      71.590  29.188  48.289  1.00 37.88      B
ATOM   1588  CG  ASN B 335      70.871  30.496  48.329  1.00 40.34      B
ATOM   1589  OD1 ASN B 335      71.266  31.422  49.033  1.00 43.76      B
ATOM   1590  ND2 ASN B 335      69.800  30.591  47.556  1.00 41.28      B
ATOM   1591  C   ASN B 335      71.292  27.070  47.013  1.00 38.24      B
ATOM   1592  O   ASN B 335      70.906  27.003  45.847  1.00 38.64      B
ATOM   1593  N   LEU B 336      72.274  26.325  47.498  1.00 36.78      B
ATOM   1594  CA  LEU B 336      72.978  25.364  46.683  1.00 35.71      B
ATOM   1595  CB  LEU B 336      74.041  24.658  47.522  1.00 35.78      B
ATOM   1596  CG  LEU B 336      74.991  23.682  46.827  1.00 35.54      B
ATOM   1597  CD1 LEU B 336      75.977  24.436  45.942  1.00 35.55      B
ATOM   1598  CD2 LEU B 336      75.716  22.899  47.883  1.00 36.31      B
ATOM   1599  C   LEU B 336      71.997  24.336  46.123  1.00 35.77      B
ATOM   1600  O   LEU B 336      72.075  23.961  44.954  1.00 37.71      B
ATOM   1601  N   LYS B 337      71.068  23.876  46.953  1.00 34.49      B
ATOM   1602  CA  LYS B 337      70.097  22.878  46.508  1.00 31.85      B
ATOM   1603  CB  LYS B 337      69.310  22.320  47.704  1.00 30.25      B
ATOM   1604  CG  LYS B 337      68.298  21.237  47.321  1.00 32.14      B
ATOM   1605  CD  LYS B 337      67.438  20.697  48.512  1.00 35.02      B
ATOM   1606  CE  LYS B 337      66.544  21.789  49.173  1.00 35.41      B
ATOM   1607  NZ  LYS B 337      65.466  21.260  50.081  1.00 32.74      B
ATOM   1608  C   LYS B 337      69.129  23.433  45.461  1.00 30.95      B
ATOM   1609  O   LYS B 337      68.793  22.740  44.519  1.00 29.84      B
ATOM   1610  N   LEU B 338      68.690  24.679  45.636  1.00 31.30      B
ATOM   1611  CA  LEU B 338      67.755  25.324  44.714  1.00 30.02      B
ATOM   1612  CB  LEU B 338      67.218  26.621  45.317  1.00 29.04      B
ATOM   1613  CG  LEU B 338      66.157  26.563  46.434  1.00 29.18      B
ATOM   1614  CD1 LEU B 338      65.834  27.996  46.909  1.00 25.48      B
ATOM   1615  CD2 LEU B 338      64.897  25.881  45.919  1.00 26.03      B
ATOM   1616  C   LEU B 338      68.433  25.639  43.400  1.00 30.20      B
ATOM   1617  O   LEU B 338      67.809  25.643  42.340  1.00 29.78      B
```

```
ATOM   1618  N   SER B 339      69.724  25.918  43.487  1.00 30.16      B
ATOM   1619  CA  SER B 339      70.510  26.227  42.317  1.00 29.06      B
ATOM   1620  CB  SER B 339      71.913  26.656  42.712  1.00 27.05      B
ATOM   1621  OG  SER B 339      72.665  26.965  41.560  1.00 25.97      B
ATOM   1622  C   SER B 339      70.598  24.979  41.483  1.00 30.90      B
ATOM   1623  O   SER B 339      70.580  25.029  40.254  1.00 32.89      B
ATOM   1624  N   GLN B 340      70.701  23.842  42.149  1.00 30.57      B
ATOM   1625  CA  GLN B 340      70.796  22.605  41.409  1.00 31.13      B
ATOM   1626  CB  GLN B 340      71.238  21.496  42.334  1.00 32.53      B
ATOM   1627  CG  GLN B 340      72.619  21.768  42.867  1.00 35.89      B
ATOM   1628  CD  GLN B 340      73.040  20.758  43.900  1.00 36.30      B
ATOM   1629  OE1 GLN B 340      72.209  19.975  44.393  1.00 37.07      B
ATOM   1630  NE2 GLN B 340      74.332  20.765  44.248  1.00 34.68      B
ATOM   1631  C   GLN B 340      69.471  22.276  40.774  1.00 31.71      B
ATOM   1632  O   GLN B 340      69.418  21.644  39.726  1.00 32.80      B
ATOM   1633  N   LYS B 341      68.403  22.738  41.408  1.00 32.39      B
ATOM   1634  CA  LYS B 341      67.047  22.505  40.942  1.00 33.18      B
ATOM   1635  CB  LYS B 341      66.086  22.760  42.094  1.00 34.86      B
ATOM   1636  CG  LYS B 341      64.697  22.223  41.889  1.00 38.21      B
ATOM   1637  CD  LYS B 341      63.793  22.574  43.061  1.00 40.03      B
ATOM   1638  CE  LYS B 341      62.406  21.980  42.836  1.00 42.58      B
ATOM   1639  NZ  LYS B 341      61.380  22.609  43.719  1.00 42.83      B
ATOM   1640  C   LYS B 341      66.661  23.392  39.764  1.00 34.36      B
ATOM   1641  O   LYS B 341      66.041  22.939  38.805  1.00 34.14      B
ATOM   1642  N   TYR B 342      67.043  24.658  39.857  1.00 34.90      B
ATOM   1643  CA  TYR B 342      66.734  25.660  38.853  1.00 35.01      B
ATOM   1644  CB  TYR B 342      65.844  26.695  39.497  1.00 37.87      B
ATOM   1645  CG  TYR B 342      64.647  26.082  40.153  1.00 41.65      B
ATOM   1646  CD1 TYR B 342      63.646  25.507  39.384  1.00 42.60      B
ATOM   1647  CE1 TYR B 342      62.525  24.958  39.968  1.00 45.40      B
ATOM   1648  CD2 TYR B 342      64.501  26.088  41.538  1.00 42.64      B
ATOM   1649  CE2 TYR B 342      63.376  25.540  42.139  1.00 44.31      B
ATOM   1650  CZ  TYR B 342      62.386  24.978  41.343  1.00 45.73      B
ATOM   1651  OH  TYR B 342      61.232  24.462  41.896  1.00 46.50      B
ATOM   1652  C   TYR B 342      67.991  26.339  38.343  1.00 34.71      B
ATOM   1653  O   TYR B 342      68.287  27.467  38.729  1.00 35.57      B
ATOM   1654  N   PRO B 343      68.754  25.663  37.474  1.00 34.09      B
ATOM   1655  CD  PRO B 343      68.568  24.298  36.955  1.00 33.06      B
ATOM   1656  CA  PRO B 343      69.982  26.256  36.942  1.00 34.15      B
ATOM   1657  CB  PRO B 343      70.427  25.231  35.902  1.00 32.61      B
ATOM   1658  CG  PRO B 343      69.940  23.953  36.458  1.00 30.81      B
ATOM   1659  C   PRO B 343      69.805  27.655  36.332  1.00 34.54      B
ATOM   1660  O   PRO B 343      70.562  28.577  36.639  1.00 34.01      B
ATOM   1661  N   LYS B 344      68.793  27.803  35.483  1.00 34.28      B
ATOM   1662  CA  LYS B 344      68.537  29.063  34.799  1.00 34.41      B
ATOM   1663  CB  LYS B 344      67.823  28.791  33.483  1.00 34.70      B
ATOM   1664  CG  LYS B 344      68.487  27.758  32.623  1.00 32.84      B
ATOM   1665  CD  LYS B 344      67.566  27.409  31.505  1.00 32.13      B
ATOM   1666  CE  LYS B 344      67.769  25.984  31.078  1.00 32.95      B
ATOM   1667  NZ  LYS B 344      66.694  25.581  30.144  1.00 35.30      B
ATOM   1668  C   LYS B 344      67.778  30.156  35.547  1.00 34.52      B
ATOM   1669  O   LYS B 344      67.446  31.188  34.950  1.00 33.51      B
ATOM   1670  N   LEU B 345      67.475  29.921  36.825  1.00 32.93      B
ATOM   1671  CA  LEU B 345      66.792  30.916  37.663  1.00 30.85      B
```

```
ATOM   1672  CB  LEU B 345      65.856  30.253  38.660  1.00 28.33      B
ATOM   1673  CG  LEU B 345      64.506  29.850  38.111  1.00 27.26      B
ATOM   1674  CD1 LEU B 345      63.691  29.121  39.179  1.00 24.62      B
ATOM   1675  CD2 LEU B 345      63.804  31.102  37.655  1.00 26.44      B
ATOM   1676  C   LEU B 345      67.834  31.674  38.440  1.00 31.07      B
ATOM   1677  O   LEU B 345      68.961  31.210  38.580  1.00 31.79      B
ATOM   1678  N   SER B 346      67.458  32.830  38.970  1.00 33.11      B
ATOM   1679  CA  SER B 346      68.392  33.653  39.754  1.00 34.10      B
ATOM   1680  CB  SER B 346      68.283  35.114  39.349  1.00 34.20      B
ATOM   1681  OG  SER B 346      67.035  35.623  39.779  1.00 37.09      B
ATOM   1682  C   SER B 346      68.098  33.563  41.247  1.00 33.12      B
ATOM   1683  O   SER B 346      66.971  33.302  41.655  1.00 33.78      B
ATOM   1684  N   GLN B 347      69.113  33.814  42.056  1.00 32.28      B
ATOM   1685  CA  GLN B 347      68.950  33.749  43.495  1.00 32.88      B
ATOM   1686  CB  GLN B 347      70.071  34.502  44.177  1.00 33.73      B
ATOM   1687  CG  GLN B 347      70.009  34.451  45.667  1.00 33.40      B
ATOM   1688  CD  GLN B 347      71.105  35.276  46.251  1.00 36.19      B
ATOM   1689  OE1 GLN B 347      71.164  36.494  46.031  1.00 38.25      B
ATOM   1690  NE2 GLN B 347      72.006  34.627  46.984  1.00 36.38      B
ATOM   1691  C   GLN B 347      67.620  34.314  43.973  1.00 31.82      B
ATOM   1692  O   GLN B 347      66.834  33.616  44.620  1.00 31.26      B
ATOM   1693  N   GLN B 348      67.370  35.581  43.661  1.00 30.61      B
ATOM   1694  CA  GLN B 348      66.121  36.195  44.076  1.00 30.85      B
ATOM   1695  CB  GLN B 348      65.984  37.626  43.542  1.00 31.61      B
ATOM   1696  CG  GLN B 348      67.092  38.583  43.958  1.00 31.41      B
ATOM   1697  CD  GLN B 348      68.291  38.552  43.014  1.00 30.33      B
ATOM   1698  OE1 GLN B 348      69.055  39.512  42.942  1.00 29.04      B
ATOM   1699  NE2 GLN B 348      68.461  37.452  42.296  1.00 29.86      B
ATOM   1700  C   GLN B 348      64.942  35.364  43.593  1.00 29.45      B
ATOM   1701  O   GLN B 348      64.183  34.831  44.400  1.00 28.92      B
ATOM   1702  N   ASP B 349      64.776  35.236  42.283  1.00 28.60      B
ATOM   1703  CA  ASP B 349      63.646  34.458  41.805  1.00 27.39      B
ATOM   1704  CB  ASP B 349      63.631  34.372  40.282  1.00 28.50      B
ATOM   1705  CG  ASP B 349      63.164  35.666  39.632  1.00 30.39      B
ATOM   1706  OD1 ASP B 349      62.212  36.306  40.153  1.00 29.22      B
ATOM   1707  OD2 ASP B 349      63.744  36.034  38.590  1.00 31.83      B
ATOM   1708  C   ASP B 349      63.571  33.061  42.404  1.00 25.37      B
ATOM   1709  O   ASP B 349      62.476  32.546  42.597  1.00 24.91      B
ATOM   1710  N   ARG B 350      64.720  32.454  42.695  1.00 22.81      B
ATOM   1711  CA  ARG B 350      64.746  31.117  43.280  1.00 21.59      B
ATOM   1712  CB  ARG B 350      66.178  30.611  43.428  1.00 23.28      B
ATOM   1713  CG  ARG B 350      66.787  30.106  42.133  1.00 27.24      B
ATOM   1714  CD  ARG B 350      68.195  29.544  42.333  1.00 26.74      B
ATOM   1715  NE  ARG B 350      68.820  29.271  41.051  1.00 27.71      B
ATOM   1716  CZ  ARG B 350      70.128  29.218  40.860  1.00 29.79      B
ATOM   1717  NH1 ARG B 350      70.956  29.416  41.878  1.00 31.36      B
ATOM   1718  NH2 ARG B 350      70.604  28.990  39.642  1.00 31.57      B
ATOM   1719  C   ARG B 350      64.094  31.124  44.651  1.00 20.94      B
ATOM   1720  O   ARG B 350      63.103  30.429  44.893  1.00 20.47      B
ATOM   1721  N   LEU B 351      64.672  31.909  45.549  1.00 18.79      B
ATOM   1722  CA  LEU B 351      64.157  32.026  46.890  1.00 17.44      B
ATOM   1723  CB  LEU B 351      64.895  33.143  47.624  1.00 14.47      B
ATOM   1724  CG  LEU B 351      66.358  32.799  47.897  1.00 14.78      B
ATOM   1725  CD1 LEU B 351      66.992  33.900  48.730  1.00 17.09      B
```

```
ATOM   1726  CD2 LEU B 351      66.466  31.467  48.619  1.00 12.98      B
ATOM   1727  C   LEU B 351      62.638  32.247  46.942  1.00 18.50      B
ATOM   1728  O   LEU B 351      61.958  31.715  47.826  1.00 17.10      B
ATOM   1729  N   ARG B 352      62.092  33.003  45.995  1.00 18.20      B
ATOM   1730  CA  ARG B 352      60.652  33.246  45.997  1.00 20.70      B
ATOM   1731  CB  ARG B 352      60.301  34.404  45.060  1.00 22.90      B
ATOM   1732  CG  ARG B 352      58.821  34.519  44.704  1.00 21.25      B
ATOM   1733  CD  ARG B 352      58.577  35.861  44.037  1.00 24.96      B
ATOM   1734  NE  ARG B 352      59.336  36.027  42.793  1.00 26.60      B
ATOM   1735  CZ  ARG B 352      58.840  35.772  41.588  1.00 24.08      B
ATOM   1736  NH1 ARG B 352      57.589  35.344  41.468  1.00 25.95      B
ATOM   1737  NH2 ARG B 352      59.582  35.955  40.508  1.00 23.94      B
ATOM   1738  C   ARG B 352      59.868  32.014  45.590  1.00 20.80      B
ATOM   1739  O   ARG B 352      58.812  31.701  46.151  1.00 20.69      B
ATOM   1740  N   LEU B 353      60.385  31.308  44.601  1.00 22.07      B
ATOM   1741  CA  LEU B 353      59.703  30.115  44.135  1.00 24.32      B
ATOM   1742  CB  LEU B 353      60.494  29.510  42.971  1.00 24.67      B
ATOM   1743  CG  LEU B 353      59.774  28.524  42.058  1.00 26.68      B
ATOM   1744  CD1 LEU B 353      59.623  27.208  42.767  1.00 28.84      B
ATOM   1745  CD2 LEU B 353      58.420  29.098  41.635  1.00 28.75      B
ATOM   1746  C   LEU B 353      59.614  29.166  45.336  1.00 25.14      B
ATOM   1747  O   LEU B 353      58.568  28.566  45.604  1.00 24.06      B
ATOM   1748  N   SER B 354      60.728  29.085  46.063  1.00 25.53      B
ATOM   1749  CA  SER B 354      60.867  28.264  47.262  1.00 26.14      B
ATOM   1750  CB  SER B 354      62.273  28.450  47.849  1.00 25.96      B
ATOM   1751  OG  SER B 354      62.454  27.730  49.061  1.00 23.97      B
ATOM   1752  C   SER B 354      59.830  28.656  48.313  1.00 27.19      B
ATOM   1753  O   SER B 354      59.098  27.818  48.837  1.00 27.24      B
ATOM   1754  N   PHE B 355      59.769  29.941  48.625  1.00 27.04      B
ATOM   1755  CA  PHE B 355      58.822  30.390  49.616  1.00 26.23      B
ATOM   1756  CB  PHE B 355      58.954  31.882  49.854  1.00 27.13      B
ATOM   1757  CG  PHE B 355      58.041  32.400  50.920  1.00 26.97      B
ATOM   1758  CD1 PHE B 355      56.736  32.763  50.626  1.00 26.60      B
ATOM   1759  CD2 PHE B 355      58.495  32.522  52.228  1.00 28.32      B
ATOM   1760  CE1 PHE B 355      55.892  33.236  51.626  1.00 27.60      B
ATOM   1761  CE2 PHE B 355      57.661  32.992  53.237  1.00 26.91      B
ATOM   1762  CZ  PHE B 355      56.360  33.353  52.934  1.00 27.81      B
ATOM   1763  C   PHE B 355      57.413  30.087  49.203  1.00 25.95      B
ATOM   1764  O   PHE B 355      56.687  29.427  49.929  1.00 25.86      B
ATOM   1765  N   LEU B 356      57.015  30.575  48.037  1.00 27.00      B
ATOM   1766  CA  LEU B 356      55.655  30.337  47.570  1.00 27.63      B
ATOM   1767  CB  LEU B 356      55.487  30.886  46.144  1.00 28.43      B
ATOM   1768  CG  LEU B 356      55.485  32.412  45.923  1.00 28.92      B
ATOM   1769  CD1 LEU B 356      55.449  32.704  44.421  1.00 28.25      B
ATOM   1770  CD2 LEU B 356      54.299  33.063  46.620  1.00 26.99      B
ATOM   1771  C   LEU B 356      55.297  28.842  47.618  1.00 26.51      B
ATOM   1772  O   LEU B 356      54.170  28.492  47.910  1.00 25.42      B
ATOM   1773  N   GLU B 357      56.267  27.976  47.343  1.00 27.82      B
ATOM   1774  CA  GLU B 357      56.051  26.537  47.357  1.00 28.89      B
ATOM   1775  CB  GLU B 357      57.223  25.841  46.668  1.00 30.18      B
ATOM   1776  CG  GLU B 357      57.193  24.319  46.727  1.00 34.82      B
ATOM   1777  CD  GLU B 357      58.032  23.659  45.640  1.00 38.48      B
ATOM   1778  OE1 GLU B 357      59.254  23.926  45.569  1.00 41.06      B
ATOM   1779  OE2 GLU B 357      57.460  22.870  44.849  1.00 40.28      B
```

```
ATOM   1780  C   GLU B 357      55.899  26.016  48.790  1.00 29.56      B
ATOM   1781  O   GLU B 357      55.055  25.165  49.072  1.00 30.56      B
ATOM   1782  N   ASN B 358      56.722  26.529  49.692  1.00 27.38      B
ATOM   1783  CA  ASN B 358      56.659  26.124  51.072  1.00 26.16      B
ATOM   1784  CB  ASN B 358      57.913  26.583  51.804  1.00 24.91      B
ATOM   1785  CG  ASN B 358      58.964  25.505  51.866  1.00 24.24      B
ATOM   1786  OD1 ASN B 358      60.149  25.794  51.827  1.00 24.48      B
ATOM   1787  ND2 ASN B 358      58.530  24.242  51.976  1.00 23.61      B
ATOM   1788  C   ASN B 358      55.440  26.669  51.796  1.00 27.01      B
ATOM   1789  O   ASN B 358      54.743  25.940  52.500  1.00 29.45      B
ATOM   1790  N   ILE B 359      55.169  27.948  51.603  1.00 25.54      B
ATOM   1791  CA  ILE B 359      54.066  28.576  52.287  1.00 24.86      B
ATOM   1792  CB  ILE B 359      53.989  30.111  51.964  1.00 23.57      B
ATOM   1793  CG2 ILE B 359      53.438  30.361  50.544  1.00 22.38      B
ATOM   1794  CG1 ILE B 359      53.099  30.808  52.994  1.00 21.88      B
ATOM   1795  CD1 ILE B 359      53.627  30.735  54.428  1.00 17.84      B
ATOM   1796  C   ILE B 359      52.726  27.929  51.992  1.00 27.18      B
ATOM   1797  O   ILE B 359      51.864  27.842  52.859  1.00 27.37      B
ATOM   1798  N   PHE B 360      52.533  27.457  50.775  1.00 29.04      B
ATOM   1799  CA  PHE B 360      51.260  26.850  50.480  1.00 30.13      B
ATOM   1800  CB  PHE B 360      50.977  26.994  48.976  1.00 31.09      B
ATOM   1801  CG  PHE B 360      50.729  28.441  48.552  1.00 35.13      B
ATOM   1802  CD1 PHE B 360      49.750  29.214  49.196  1.00 36.04      B
ATOM   1803  CD2 PHE B 360      51.480  29.040  47.540  1.00 35.99      B
ATOM   1804  CE1 PHE B 360      49.531  30.554  48.837  1.00 36.47      B
ATOM   1805  CE2 PHE B 360      51.265  30.380  47.177  1.00 37.16      B
ATOM   1806  CZ  PHE B 360      50.290  31.138  47.827  1.00 35.98      B
ATOM   1807  C   PHE B 360      51.137  25.414  51.019  1.00 28.89      B
ATOM   1808  O   PHE B 360      50.040  24.932  51.282  1.00 29.91      B
ATOM   1809  N   ILE B 361      52.258  24.739  51.221  1.00 26.91      B
ATOM   1810  CA  ILE B 361      52.212  23.405  51.799  1.00 25.90      B
ATOM   1811  CB  ILE B 361      53.567  22.687  51.626  1.00 24.75      B
ATOM   1812  CG2 ILE B 361      53.707  21.556  52.648  1.00 20.19      B
ATOM   1813  CG1 ILE B 361      53.695  22.198  50.187  1.00 21.38      B
ATOM   1814  CD1 ILE B 361      55.017  21.579  49.880  1.00 21.49      B
ATOM   1815  C   ILE B 361      51.894  23.539  53.303  1.00 25.76      B
ATOM   1816  O   ILE B 361      51.165  22.724  53.854  1.00 25.25      B
ATOM   1817  N   LEU B 362      52.455  24.558  53.955  1.00 24.78      B
ATOM   1818  CA  LEU B 362      52.200  24.780  55.367  1.00 24.80      B
ATOM   1819  CB  LEU B 362      53.097  25.890  55.942  1.00 24.95      B
ATOM   1820  CG  LEU B 362      52.861  26.232  57.439  1.00 25.61      B
ATOM   1821  CD1 LEU B 362      53.251  25.034  58.290  1.00 23.05      B
ATOM   1822  CD2 LEU B 362      53.682  27.448  57.891  1.00 24.66      B
ATOM   1823  C   LEU B 362      50.746  25.192  55.479  1.00 24.68      B
ATOM   1824  O   LEU B 362      50.075  24.847  56.440  1.00 25.14      B
ATOM   1825  N   LYS B 363      50.262  25.932  54.485  1.00 26.90      B
ATOM   1826  CA  LYS B 363      48.870  26.397  54.455  1.00 28.18      B
ATOM   1827  CB  LYS B 363      48.607  27.192  53.178  1.00 30.22      B
ATOM   1828  CG  LYS B 363      48.946  28.677  53.262  1.00 34.21      B
ATOM   1829  CD  LYS B 363      47.787  29.466  53.860  1.00 35.29      B
ATOM   1830  CE  LYS B 363      48.036  30.984  53.859  1.00 38.15      B
ATOM   1831  NZ  LYS B 363      48.196  31.608  52.486  1.00 38.16      B
ATOM   1832  C   LYS B 363      47.931  25.209  54.497  1.00 27.14      B
ATOM   1833  O   LYS B 363      46.852  25.288  55.076  1.00 27.91      B
```

```
ATOM   1834  N   ASN B 364      48.365  24.119  53.872  1.00 26.50      B
ATOM   1835  CA  ASN B 364      47.602  22.893  53.809  1.00 28.02      B
ATOM   1836  CB  ASN B 364      48.119  21.990  52.692  1.00 29.30      B
ATOM   1837  CG  ASN B 364      47.742  22.485  51.311  1.00 30.37      B
ATOM   1838  OD1 ASN B 364      48.127  21.882  50.299  1.00 29.53      B
ATOM   1839  ND2 ASN B 364      46.982  23.584  51.255  1.00 31.60      B
ATOM   1840  C   ASN B 364      47.696  22.129  55.106  1.00 27.69      B
ATOM   1841  O   ASN B 364      46.716  21.551  55.559  1.00 28.47      B
ATOM   1842  N   TRP B 365      48.882  22.093  55.693  1.00 26.51      B
ATOM   1843  CA  TRP B 365      49.039  21.371  56.938  1.00 27.73      B
ATOM   1844  CB  TRP B 365      50.489  21.397  57.400  1.00 29.20      B
ATOM   1845  CG  TRP B 365      51.351  20.381  56.790  1.00 29.13      B
ATOM   1846  CD2 TRP B 365      51.742  19.142  57.379  1.00 29.19      B
ATOM   1847  CE2 TRP B 365      52.638  18.523  56.489  1.00 28.54      B
ATOM   1848  CE3 TRP B 365      51.425  18.495  58.579  1.00 29.88      B
ATOM   1849  CD1 TRP B 365      51.989  20.460  55.598  1.00 28.45      B
ATOM   1850  NE1 TRP B 365      52.771  19.351  55.406  1.00 27.81      B
ATOM   1851  CZ2 TRP B 365      53.230  17.282  56.758  1.00 28.80      B
ATOM   1852  CZ3 TRP B 365      52.018  17.257  58.842  1.00 29.52      B
ATOM   1853  CH2 TRP B 365      52.909  16.671  57.934  1.00 27.59      B
ATOM   1854  C   TRP B 365      48.183  21.976  58.037  1.00 27.25      B
ATOM   1855  O   TRP B 365      47.686  21.262  58.898  1.00 27.54      B
ATOM   1856  N   TYR B 366      48.015  23.293  57.985  1.00 25.59      B
ATOM   1857  CA  TYR B 366      47.271  24.038  58.989  1.00 25.83      B
ATOM   1858  CB  TYR B 366      47.858  25.433  59.127  1.00 24.61      B
ATOM   1859  CG  TYR B 366      49.220  25.559  59.761  1.00 22.97      B
ATOM   1860  CD1 TYR B 366      49.803  24.511  60.469  1.00 23.61      B
ATOM   1861  CE1 TYR B 366      50.999  24.699  61.170  1.00 21.04      B
ATOM   1862  CD2 TYR B 366      49.871  26.779  59.760  1.00 21.89      B
ATOM   1863  CE2 TYR B 366      51.050  26.968  60.452  1.00 20.89      B
ATOM   1864  CZ  TYR B 366      51.603  25.940  61.153  1.00 20.92      B
ATOM   1865  OH  TYR B 366      52.741  26.179  61.878  1.00 21.34      B
ATOM   1866  C   TYR B 366      45.781  24.205  58.730  1.00 26.75      B
ATOM   1867  O   TYR B 366      45.053  24.659  59.618  1.00 25.47      B
ATOM   1868  N   ASN B 367      45.343  23.874  57.516  1.00 27.78      B
ATOM   1869  CA  ASN B 367      43.935  23.993  57.137  1.00 28.96      B
ATOM   1870  CB  ASN B 367      43.789  24.062  55.611  1.00 27.81      B
ATOM   1871  CG  ASN B 367      42.420  24.542  55.172  1.00 27.70      B
ATOM   1872  OD1 ASN B 367      41.462  24.533  55.944  1.00 29.38      B
ATOM   1873  ND2 ASN B 367      42.321  24.957  53.915  1.00 27.06      B
ATOM   1874  C   ASN B 367      43.184  22.772  57.668  1.00 29.83      B
ATOM   1875  O   ASN B 367      43.454  21.638  57.253  1.00 30.52      B
ATOM   1876  N   PRO B 368      42.246  22.988  58.613  1.00 30.10      B
ATOM   1877  CD  PRO B 368      41.884  24.278  59.227  1.00 28.86      B
ATOM   1878  CA  PRO B 368      41.458  21.889  59.200  1.00 29.62      B
ATOM   1879  CB  PRO B 368      40.654  22.578  60.304  1.00 28.09      B
ATOM   1880  CG  PRO B 368      41.398  23.839  60.573  1.00 28.33      B
ATOM   1881  C   PRO B 368      40.534  21.318  58.133  1.00 29.34      B
ATOM   1882  O   PRO B 368      40.223  20.133  58.118  1.00 28.44      B
ATOM   1883  N   LYS B 369      40.083  22.202  57.256  1.00 29.08      B
ATOM   1884  CA  LYS B 369      39.202  21.814  56.187  1.00 30.72      B
ATOM   1885  CB  LYS B 369      38.417  23.044  55.697  1.00 32.78      B
ATOM   1886  CG  LYS B 369      37.095  23.310  56.487  1.00 34.07      B
ATOM   1887  CD  LYS B 369      36.649  24.778  56.462  1.00 36.76      B
```

```
ATOM   1888  CE  LYS B 369      36.882  25.442  55.098  1.00 38.43      B
ATOM   1889  NZ  LYS B 369      36.568  26.906  55.151  1.00 41.21      B
ATOM   1890  C   LYS B 369      39.977  21.145  55.050  1.00 30.60      B
ATOM   1891  O   LYS B 369      39.389  20.779  54.040  1.00 32.44      B
ATOM   1892  N   PHE B 370      41.293  20.985  55.207  1.00 29.96      B
ATOM   1893  CA  PHE B 370      42.111  20.335  54.175  1.00 28.15      B
ATOM   1894  CB  PHE B 370      43.422  21.107  53.934  1.00 29.31      B
ATOM   1895  CG  PHE B 370      44.447  20.330  53.124  1.00 31.81      B
ATOM   1896  CD1 PHE B 370      45.283  19.394  53.738  1.00 34.71      B
ATOM   1897  CD2 PHE B 370      44.536  20.484  51.745  1.00 31.92      B
ATOM   1898  CE1 PHE B 370      46.185  18.625  52.992  1.00 34.80      B
ATOM   1899  CE2 PHE B 370      45.436  19.718  50.992  1.00 33.21      B
ATOM   1900  CZ  PHE B 370      46.259  18.785  51.622  1.00 33.35      B
ATOM   1901  C   PHE B 370      42.431  18.886  54.537  1.00 26.13      B
ATOM   1902  O   PHE B 370      42.750  18.584  55.682  1.00 26.19      B
ATOM   1903  N   VAL B 371      42.352  17.993  53.556  1.00 25.26      B
ATOM   1904  CA  VAL B 371      42.656  16.590  53.811  1.00 24.76      B
ATOM   1905  CB  VAL B 371      41.419  15.694  53.697  1.00 25.22      B
ATOM   1906  CG1 VAL B 371      41.736  14.297  54.237  1.00 22.91      B
ATOM   1907  CG2 VAL B 371      40.257  16.324  54.442  1.00 23.49      B
ATOM   1908  C   VAL B 371      43.712  16.062  52.863  1.00 24.14      B
ATOM   1909  O   VAL B 371      43.585  16.188  51.653  1.00 23.89      B
ATOM   1910  N   PRO B 372      44.767  15.447  53.418  1.00 24.76      B
ATOM   1911  CD  PRO B 372      44.861  15.087  54.840  1.00 25.65      B
ATOM   1912  CA  PRO B 372      45.889  14.878  52.678  1.00 25.57      B
ATOM   1913  CB  PRO B 372      46.835  14.390  53.769  1.00 25.32      B
ATOM   1914  CG  PRO B 372      46.318  14.998  55.041  1.00 26.54      B
ATOM   1915  C   PRO B 372      45.421  13.720  51.863  1.00 27.92      B
ATOM   1916  O   PRO B 372      44.359  13.144  52.143  1.00 29.78      B
ATOM   1917  N   GLN B 373      46.223  13.375  50.858  1.00 28.98      B
ATOM   1918  CA  GLN B 373      45.940  12.222  50.002  1.00 29.41      B
ATOM   1919  CB  GLN B 373      46.566  12.412  48.600  1.00 29.51      B
ATOM   1920  CG  GLN B 373      45.660  13.145  47.586  1.00 29.73      B
ATOM   1921  CD  GLN B 373      46.354  13.455  46.247  1.00 30.26      B
ATOM   1922  OE1 GLN B 373      47.091  14.429  46.129  1.00 30.70      B
ATOM   1923  NE2 GLN B 373      46.113  12.621  45.240  1.00 30.61      B
ATOM   1924  C   GLN B 373      46.554  11.029  50.758  1.00 28.67      B
ATOM   1925  O   GLN B 373      47.662  11.119  51.274  1.00 28.24      B
ATOM   1926  N   ARG B 374      45.803   9.936  50.845  1.00 28.06      B
ATOM   1927  CA  ARG B 374      46.213   8.728  51.557  1.00 25.68      B
ATOM   1928  CB  ARG B 374      45.030   8.254  52.416  1.00 25.68      B
ATOM   1929  CG  ARG B 374      45.173   6.929  53.159  1.00 24.87      B
ATOM   1930  CD  ARG B 374      45.727   7.099  54.544  1.00 25.14      B
ATOM   1931  NE  ARG B 374      45.604   5.872  55.347  1.00 26.59      B
ATOM   1932  CZ  ARG B 374      44.549   5.554  56.099  1.00 24.91      B
ATOM   1933  NH1 ARG B 374      43.503   6.370  56.171  1.00 23.91      B
ATOM   1934  NH2 ARG B 374      44.533   4.407  56.770  1.00 23.39      B
ATOM   1935  C   ARG B 374      46.650   7.619  50.598  1.00 25.60      B
ATOM   1936  O   ARG B 374      45.978   7.352  49.591  1.00 25.61      B
ATOM   1937  N   THR B 375      47.790   7.000  50.909  1.00 24.83      B
ATOM   1938  CA  THR B 375      48.325   5.895  50.124  1.00 24.29      B
ATOM   1939  CB  THR B 375      49.562   6.298  49.278  1.00 24.62      B
ATOM   1940  OG1 THR B 375      49.334   7.559  48.630  1.00 26.27      B
ATOM   1941  CG2 THR B 375      49.845   5.228  48.217  1.00 22.20      B
```

```
ATOM   1942  C   THR B 375      48.787   4.844  51.125  1.00 25.05      B
ATOM   1943  O   THR B 375      49.710   5.108  51.889  1.00 25.56      B
ATOM   1944  N   THR B 376      48.149   3.669  51.122  1.00 25.33      B
ATOM   1945  CA  THR B 376      48.509   2.571  52.034  1.00 25.61      B
ATOM   1946  CB  THR B 376      47.254   1.951  52.733  1.00 23.00      B
ATOM   1947  OG1 THR B 376      46.361   2.992  53.148  1.00 23.90      B
ATOM   1948  CG2 THR B 376      47.678   1.125  53.956  1.00 21.63      B
ATOM   1949  C   THR B 376      49.224   1.439  51.273  1.00 27.50      B
ATOM   1950  O   THR B 376      48.696   0.916  50.303  1.00 27.69      B
ATOM   1951  N   LEU B 377      50.413   1.058  51.735  1.00 29.38      B
ATOM   1952  CA  LEU B 377      51.204  -0.001  51.119  1.00 29.82      B
ATOM   1953  CB  LEU B 377      52.540   0.574  50.650  1.00 27.89      B
ATOM   1954  CG  LEU B 377      52.396   1.871  49.837  1.00 27.64      B
ATOM   1955  CD1 LEU B 377      53.754   2.507  49.549  1.00 23.10      B
ATOM   1956  CD2 LEU B 377      51.643   1.570  48.562  1.00 26.07      B
ATOM   1957  C   LEU B 377      51.451  -1.131  52.125  1.00 32.73      B
ATOM   1958  O   LEU B 377      51.328  -0.925  53.327  1.00 32.89      B
ATOM   1959  N   ARG B 378      51.815  -2.315  51.633  1.00 36.51      B
ATOM   1960  CA  ARG B 378      52.071  -3.463  52.498  1.00 39.20      B
ATOM   1961  CB  ARG B 378      52.180  -4.757  51.678  1.00 42.06      B
ATOM   1962  CG  ARG B 378      52.510  -6.019  52.506  1.00 45.42      B
ATOM   1963  CD  ARG B 378      52.472  -7.335  51.682  1.00 48.17      B
ATOM   1964  NE  ARG B 378      51.210  -7.513  50.958  1.00 51.30      B
ATOM   1965  CZ  ARG B 378      50.850  -8.616  50.306  1.00 52.70      B
ATOM   1966  NH1 ARG B 378      51.655  -9.673  50.281  1.00 53.25      B
ATOM   1967  NH2 ARG B 378      49.684  -8.654  49.664  1.00 54.26      B
ATOM   1968  C   ARG B 378      53.333  -3.278  53.307  1.00 40.74      B
ATOM   1969  O   ARG B 378      54.339  -2.747  52.819  1.00 40.15      B
ATOM   1970  N   GLY B 379      53.266  -3.735  54.555  1.00 42.99      B
ATOM   1971  CA  GLY B 379      54.394  -3.628  55.463  1.00 43.31      B
ATOM   1972  C   GLY B 379      55.221  -4.897  55.532  1.00 43.80      B
ATOM   1973  O   GLY B 379      55.501  -5.532  54.516  1.00 42.41      B
ATOM   1974  N   HIS B 380      55.609  -5.264  56.747  1.00 44.62      B
ATOM   1975  CA  HIS B 380      56.421  -6.451  56.972  1.00 45.57      B
ATOM   1976  CB  HIS B 380      57.468  -6.163  58.049  1.00 42.95      B
ATOM   1977  CG  HIS B 380      58.489  -5.148  57.640  1.00 41.43      B
ATOM   1978  CD2 HIS B 380      58.369  -3.842  57.307  1.00 39.61      B
ATOM   1979  ND1 HIS B 380      59.833  -5.444  57.559  1.00 40.42      B
ATOM   1980  CE1 HIS B 380      60.497  -4.362  57.195  1.00 39.52      B
ATOM   1981  NE2 HIS B 380      59.633  -3.376  57.037  1.00 39.67      B
ATOM   1982  C   HIS B 380      55.552  -7.627  57.398  1.00 47.13      B
ATOM   1983  O   HIS B 380      54.374  -7.457  57.690  1.00 47.01      B
ATOM   1984  N   MSE B 381      56.127  -8.822  57.440  1.00 49.63      B
ATOM   1985  CA  MSE B 381      55.350  -9.979  57.826  1.00 51.34      B
ATOM   1986  CB  MSE B 381      56.181 -11.238  57.658  1.00 54.42      B
ATOM   1987  CG  MSE B 381      56.131 -11.740  56.225  1.00 60.08      B
ATOM   1988  SE  MSE B 381      57.583 -12.923  55.737  1.00 69.56      B
ATOM   1989  CE  MSE B 381      56.901 -14.517  56.629  1.00 64.33      B
ATOM   1990  C   MSE B 381      54.800  -9.860  59.227  1.00 51.47      B
ATOM   1991  O   MSE B 381      53.645 -10.193  59.464  1.00 53.52      B
ATOM   1992  N   THR B 382      55.608  -9.366  60.158  1.00 50.41      B
ATOM   1993  CA  THR B 382      55.159  -9.204  61.539  1.00 48.29      B
ATOM   1994  CB  THR B 382      56.367  -9.222  62.513  1.00 48.92      B
ATOM   1995  OG1 THR B 382      55.931  -8.858  63.825  1.00 49.73      B
```

```
ATOM   1996  CG2 THR B 382      57.457  -8.259  62.048  1.00 51.19      B
ATOM   1997  C   THR B 382      54.361  -7.903  61.674  1.00 46.73      B
ATOM   1998  O   THR B 382      54.511  -6.990  60.858  1.00 45.72      B
ATOM   1999  N   SER B 383      53.510  -7.818  62.695  1.00 45.75      B
ATOM   2000  CA  SER B 383      52.667  -6.631  62.888  1.00 44.00      B
ATOM   2001  CB  SER B 383      51.418  -6.988  63.706  1.00 44.17      B
ATOM   2002  OG  SER B 383      51.707  -6.998  65.093  1.00 44.67      B
ATOM   2003  C   SER B 383      53.363  -5.440  63.552  1.00 42.52      B
ATOM   2004  O   SER B 383      52.739  -4.400  63.769  1.00 42.16      B
ATOM   2005  N   VAL B 384      54.645  -5.584  63.875  1.00 40.61      B
ATOM   2006  CA  VAL B 384      55.368  -4.496  64.519  1.00 38.88      B
ATOM   2007  CB  VAL B 384      55.785  -4.868  65.971  1.00 37.56      B
ATOM   2008  CG1 VAL B 384      56.490  -3.706  66.635  1.00 34.97      B
ATOM   2009  CG2 VAL B 384      54.570  -5.273  66.772  1.00 37.83      B
ATOM   2010  C   VAL B 384      56.617  -4.090  63.756  1.00 38.38      B
ATOM   2011  O   VAL B 384      57.507  -4.906  63.506  1.00 38.18      B
ATOM   2012  N   ILE B 385      56.674  -2.823  63.372  1.00 37.92      B
ATOM   2013  CA  ILE B 385      57.842  -2.330  62.674  1.00 38.47      B
ATOM   2014  CB  ILE B 385      57.462  -1.284  61.570  1.00 38.37      B
ATOM   2015  CG2 ILE B 385      58.692  -0.795  60.853  1.00 35.43      B
ATOM   2016  CG1 ILE B 385      56.610  -1.951  60.483  1.00 38.29      B
ATOM   2017  CD1 ILE B 385      56.296  -1.048  59.293  1.00 40.13      B
ATOM   2018  C   ILE B 385      58.752  -1.744  63.758  1.00 38.62      B
ATOM   2019  O   ILE B 385      58.295  -1.054  64.679  1.00 39.76      B
ATOM   2020  N   THR B 386      60.040  -2.057  63.649  1.00 37.77      B
ATOM   2021  CA  THR B 386      61.053  -1.643  64.616  1.00 34.37      B
ATOM   2022  CB  THR B 386      62.142  -2.722  64.734  1.00 32.81      B
ATOM   2023  OG1 THR B 386      62.810  -2.855  63.473  1.00 31.89      B
ATOM   2024  CG2 THR B 386      61.528  -4.050  65.098  1.00 32.45      B
ATOM   2025  C   THR B 386      61.740  -0.329  64.281  1.00 32.70      B
ATOM   2026  O   THR B 386      62.088   0.438  65.167  1.00 33.06      B
ATOM   2027  N   CYS B 387      61.947  -0.058  63.005  1.00 31.07      B
ATOM   2028  CA  CYS B 387      62.627   1.178  62.659  1.00 30.70      B
ATOM   2029  CB  CYS B 387      64.140   0.964  62.769  1.00 29.49      B
ATOM   2030  SG  CYS B 387      64.707  -0.568  62.008  1.00 32.59      B
ATOM   2031  C   CYS B 387      62.250   1.702  61.268  1.00 29.94      B
ATOM   2032  O   CYS B 387      61.896   0.927  60.365  1.00 27.25      B
ATOM   2033  N   LEU B 388      62.349   3.021  61.097  1.00 29.32      B
ATOM   2034  CA  LEU B 388      62.001   3.659  59.828  1.00 28.34      B
ATOM   2035  CB  LEU B 388      60.534   4.097  59.878  1.00 28.15      B
ATOM   2036  CG  LEU B 388      59.848   4.716  58.662  1.00 25.84      B
ATOM   2037  CD1 LEU B 388      58.358   4.729  58.925  1.00 26.04      B
ATOM   2038  CD2 LEU B 388      60.361   6.117  58.401  1.00 24.86      B
ATOM   2039  C   LEU B 388      62.885   4.851  59.479  1.00 26.75      B
ATOM   2040  O   LEU B 388      63.211   5.661  60.336  1.00 25.66      B
ATOM   2041  N   GLN B 389      63.284   4.947  58.214  1.00 27.43      B
ATOM   2042  CA  GLN B 389      64.112   6.067  57.753  1.00 27.85      B
ATOM   2043  CB  GLN B 389      65.505   5.589  57.308  1.00 28.80      B
ATOM   2044  CG  GLN B 389      66.450   5.215  58.443  1.00 29.07      B
ATOM   2045  CD  GLN B 389      66.900   6.425  59.249  1.00 29.82      B
ATOM   2046  OE1 GLN B 389      67.815   7.152  58.849  1.00 30.35      B
ATOM   2047  NE2 GLN B 389      66.244   6.654  60.383  1.00 27.50      B
ATOM   2048  C   GLN B 389      63.417   6.718  56.577  1.00 26.75      B
ATOM   2049  O   GLN B 389      62.792   6.035  55.766  1.00 26.92      B
```

ATOM	2050	N	PHE	B	390	63.532	8.037	56.483	1.00	26.42	B
ATOM	2051	CA	PHE	B	390	62.928	8.778	55.382	1.00	26.53	B
ATOM	2052	CB	PHE	B	390	61.606	9.405	55.833	1.00	24.52	B
ATOM	2053	CG	PHE	B	390	60.846	10.069	54.728	1.00	23.83	B
ATOM	2054	CD1	PHE	B	390	60.614	9.408	53.530	1.00	24.31	B
ATOM	2055	CD2	PHE	B	390	60.357	11.358	54.883	1.00	24.82	B
ATOM	2056	CE1	PHE	B	390	59.906	10.021	52.496	1.00	24.43	B
ATOM	2057	CE2	PHE	B	390	59.643	11.985	53.851	1.00	26.18	B
ATOM	2058	CZ	PHE	B	390	59.418	11.316	52.657	1.00	25.05	B
ATOM	2059	C	PHE	B	390	63.885	9.852	54.853	1.00	28.00	B
ATOM	2060	O	PHE	B	390	64.003	10.930	55.439	1.00	26.52	B
ATOM	2061	N	GLU	B	391	64.591	9.532	53.761	1.00	31.44	B
ATOM	2062	CA	GLU	B	391	65.552	10.459	53.112	1.00	34.19	B
ATOM	2063	CB	GLU	B	391	66.958	10.374	53.753	1.00	35.50	B
ATOM	2064	CG	GLU	B	391	67.082	9.731	55.143	1.00	38.57	B
ATOM	2065	CD	GLU	B	391	66.652	10.654	56.306	1.00	40.82	B
ATOM	2066	OE1	GLU	B	391	66.842	11.896	56.199	1.00	38.26	B
ATOM	2067	OE2	GLU	B	391	66.138	10.116	57.327	1.00	41.64	B
ATOM	2068	C	GLU	B	391	65.706	10.165	51.602	1.00	34.30	B
ATOM	2069	O	GLU	B	391	65.415	9.060	51.141	1.00	32.53	B
ATOM	2070	N	ASP	B	392	66.179	11.151	50.842	1.00	35.27	B
ATOM	2071	CA	ASP	B	392	66.388	10.979	49.395	1.00	35.87	B
ATOM	2072	CB	ASP	B	392	67.633	10.114	49.106	1.00	35.92	B
ATOM	2073	CG	ASP	B	392	68.941	10.886	49.139	1.00	36.64	B
ATOM	2074	OD1	ASP	B	392	68.967	12.093	48.795	1.00	37.84	B
ATOM	2075	OD2	ASP	B	392	69.964	10.253	49.492	1.00	36.21	B
ATOM	2076	C	ASP	B	392	65.215	10.300	48.673	1.00	36.11	B
ATOM	2077	O	ASP	B	392	65.452	9.465	47.805	1.00	36.71	B
ATOM	2078	N	ASN	B	393	63.968	10.618	49.018	1.00	35.71	B
ATOM	2079	CA	ASN	B	393	62.805	9.999	48.347	1.00	35.51	B
ATOM	2080	CB	ASN	B	393	62.861	10.281	46.847	1.00	34.88	B
ATOM	2081	CG	ASN	B	393	62.762	11.755	46.544	1.00	37.09	B
ATOM	2082	OD1	ASN	B	393	61.672	12.328	46.584	1.00	36.85	B
ATOM	2083	ND2	ASN	B	393	63.903	12.388	46.255	1.00	37.57	B
ATOM	2084	C	ASN	B	393	62.633	8.489	48.570	1.00	35.26	B
ATOM	2085	O	ASN	B	393	61.925	7.805	47.817	1.00	34.05	B
ATOM	2086	N	TYR	B	394	63.283	7.990	49.618	1.00	35.44	B
ATOM	2087	CA	TYR	B	394	63.246	6.585	50.004	1.00	33.92	B
ATOM	2088	CB	TYR	B	394	64.660	6.006	50.087	1.00	34.53	B
ATOM	2089	CG	TYR	B	394	65.314	5.705	48.772	1.00	35.08	B
ATOM	2090	CD1	TYR	B	394	64.808	4.707	47.944	1.00	33.82	B
ATOM	2091	CE1	TYR	B	394	65.424	4.394	46.753	1.00	35.67	B
ATOM	2092	CD2	TYR	B	394	66.461	6.393	48.370	1.00	33.92	B
ATOM	2093	CE2	TYR	B	394	67.093	6.091	47.179	1.00	36.23	B
ATOM	2094	CZ	TYR	B	394	66.571	5.090	46.369	1.00	37.49	B
ATOM	2095	OH	TYR	B	394	67.184	4.785	45.167	1.00	39.46	B
ATOM	2096	C	TYR	B	394	62.652	6.473	51.393	1.00	33.94	B
ATOM	2097	O	TYR	B	394	62.973	7.268	52.281	1.00	32.72	B
ATOM	2098	N	VAL	B	395	61.804	5.470	51.575	1.00	33.59	B
ATOM	2099	CA	VAL	B	395	61.200	5.196	52.864	1.00	33.27	B
ATOM	2100	CB	VAL	B	395	59.655	5.170	52.787	1.00	33.84	B
ATOM	2101	CG1	VAL	B	395	59.055	4.927	54.167	1.00	32.25	B
ATOM	2102	CG2	VAL	B	395	59.145	6.467	52.213	1.00	34.69	B
ATOM	2103	C	VAL	B	395	61.708	3.803	53.182	1.00	33.68	B

ATOM	2104	O	VAL	B	395	61.334	2.822	52.526	1.00	35.51	B
ATOM	2105	N	ILE	B	396	62.592	3.701	54.163	1.00	33.52	B
ATOM	2106	CA	ILE	B	396	63.113	2.386	54.508	1.00	32.85	B
ATOM	2107	CB	ILE	B	396	64.666	2.403	54.579	1.00	33.18	B
ATOM	2108	CG2	ILE	B	396	65.207	0.998	54.438	1.00	32.95	B
ATOM	2109	CG1	ILE	B	396	65.238	3.231	53.434	1.00	32.57	B
ATOM	2110	CD1	ILE	B	396	66.704	3.519	53.594	1.00	34.98	B
ATOM	2111	C	ILE	B	396	62.527	1.999	55.862	1.00	30.96	B
ATOM	2112	O	ILE	B	396	62.550	2.787	56.805	1.00	29.47	B
ATOM	2113	N	THR	B	397	61.977	0.792	55.943	1.00	29.81	B
ATOM	2114	CA	THR	B	397	61.397	0.303	57.188	1.00	30.52	B
ATOM	2115	CB	THR	B	397	59.883	0.014	57.087	1.00	28.68	B
ATOM	2116	OG1	THR	B	397	59.685	-1.096	56.216	1.00	27.52	B
ATOM	2117	CG2	THR	B	397	59.127	1.206	56.561	1.00	28.88	B
ATOM	2118	C	THR	B	397	62.052	-1.012	57.574	1.00	32.66	B
ATOM	2119	O	THR	B	397	62.495	-1.768	56.708	1.00	32.93	B
ATOM	2120	N	GLY	B	398	62.095	-1.283	58.878	1.00	34.04	B
ATOM	2121	CA	GLY	B	398	62.673	-2.521	59.377	1.00	36.31	B
ATOM	2122	C	GLY	B	398	61.790	-3.205	60.409	1.00	38.57	B
ATOM	2123	O	GLY	B	398	61.203	-2.535	61.257	1.00	38.84	B
ATOM	2124	N	ALA	B	399	61.692	-4.532	60.347	1.00	40.48	B
ATOM	2125	CA	ALA	B	399	60.870	-5.274	61.304	1.00	43.09	B
ATOM	2126	CB	ALA	B	399	59.540	-5.687	60.660	1.00	43.54	B
ATOM	2127	C	ALA	B	399	61.577	-6.506	61.870	1.00	44.04	B
ATOM	2128	O	ALA	B	399	62.688	-6.838	61.461	1.00	43.75	B
ATOM	2129	N	ASP	B	400	60.921	-7.182	62.811	1.00	45.72	B
ATOM	2130	CA	ASP	B	400	61.498	-8.363	63.446	1.00	47.39	B
ATOM	2131	CB	ASP	B	400	60.854	-8.596	64.820	1.00	48.07	B
ATOM	2132	CG	ASP	B	400	61.569	-9.666	65.626	1.00	48.91	B
ATOM	2133	OD1	ASP	B	400	62.791	-9.515	65.869	1.00	49.38	B
ATOM	2134	OD2	ASP	B	400	60.910	-10.656	66.012	1.00	48.62	B
ATOM	2135	C	ASP	B	400	61.347	-9.610	62.579	1.00	47.48	B
ATOM	2136	O	ASP	B	400	61.522	-10.735	63.048	1.00	49.06	B
ATOM	2137	N	ASP	B	401	61.014	-9.403	61.313	1.00	46.02	B
ATOM	2138	CA	ASP	B	401	60.851	-10.501	60.378	1.00	43.80	B
ATOM	2139	CB	ASP	B	401	59.688	-10.192	59.436	1.00	45.11	B
ATOM	2140	CG	ASP	B	401	59.962	-8.996	58.541	1.00	46.35	B
ATOM	2141	OD1	ASP	B	401	60.797	-8.130	58.909	1.00	46.25	B
ATOM	2142	OD2	ASP	B	401	59.325	-8.919	57.465	1.00	47.47	B
ATOM	2143	C	ASP	B	401	62.147	-10.661	59.592	1.00	42.18	B
ATOM	2144	O	ASP	B	401	62.153	-11.209	58.498	1.00	40.84	B
ATOM	2145	N	LYS	B	402	63.241	-10.171	60.174	1.00	42.03	B
ATOM	2146	CA	LYS	B	402	64.581	-10.221	59.577	1.00	41.37	B
ATOM	2147	CB	LYS	B	402	65.061	-11.671	59.394	1.00	41.89	B
ATOM	2148	CG	LYS	B	402	64.777	-12.595	60.546	1.00	40.16	B
ATOM	2149	CD	LYS	B	402	65.248	-14.004	60.249	1.00	39.21	B
ATOM	2150	CE	LYS	B	402	64.973	-14.910	61.453	1.00	41.18	B
ATOM	2151	NZ	LYS	B	402	65.506	-16.306	61.313	1.00	41.31	B
ATOM	2152	C	LYS	B	402	64.584	-9.545	58.217	1.00	41.18	B
ATOM	2153	O	LYS	B	402	65.387	-9.880	57.350	1.00	41.03	B
ATOM	2154	N	MSE	B	403	63.700	-8.583	58.021	1.00	41.52	B
ATOM	2155	CA	MSE	B	403	63.643	-7.932	56.731	1.00	41.52	B
ATOM	2156	CB	MSE	B	403	62.364	-8.354	56.024	1.00	44.20	B
ATOM	2157	CG	MSE	B	403	62.593	-8.927	54.649	1.00	49.51	B

```
ATOM   2158  SE  MSE B 403      63.401 -10.704  54.630  1.00 56.96      B
ATOM   2159  CE  MSE B 403      61.754 -11.724  54.910  1.00 52.63      B
ATOM   2160  C   MSE B 403      63.728  -6.408  56.765  1.00 39.82      B
ATOM   2161  O   MSE B 403      63.396  -5.758  57.763  1.00 39.40      B
ATOM   2162  N   ILE B 404      64.163  -5.861  55.638  1.00 37.19      B
ATOM   2163  CA  ILE B 404      64.305  -4.432  55.441  1.00 34.55      B
ATOM   2164  CB  ILE B 404      65.790  -4.049  55.290  1.00 33.79      B
ATOM   2165  CG2 ILE B 404      65.904  -2.619  54.750  1.00 32.01      B
ATOM   2166  CG1 ILE B 404      66.516  -4.256  56.628  1.00 32.98      B
ATOM   2167  CD1 ILE B 404      68.003  -3.868  56.634  1.00 32.54      B
ATOM   2168  C   ILE B 404      63.576  -4.060  54.152  1.00 34.51      B
ATOM   2169  O   ILE B 404      63.994  -4.455  53.061  1.00 33.17      B
ATOM   2170  N   ARG B 405      62.489  -3.303  54.275  1.00 34.07      B
ATOM   2171  CA  ARG B 405      61.714  -2.890  53.104  1.00 34.11      B
ATOM   2172  CB  ARG B 405      60.222  -3.145  53.349  1.00 31.76      B
ATOM   2173  CG  ARG B 405      59.877  -4.612  53.569  1.00 29.64      B
ATOM   2174  CD  ARG B 405      58.419  -4.820  53.979  1.00 28.14      B
ATOM   2175  NE  ARG B 405      57.449  -4.457  52.948  1.00 28.57      B
ATOM   2176  CZ  ARG B 405      57.252  -5.129  51.813  1.00 28.90      B
ATOM   2177  NH1 ARG B 405      57.964  -6.215  51.537  1.00 25.04      B
ATOM   2178  NH2 ARG B 405      56.311  -4.728  50.960  1.00 29.02      B
ATOM   2179  C   ARG B 405      61.912  -1.425  52.730  1.00 34.97      B
ATOM   2180  O   ARG B 405      61.823  -0.545  53.580  1.00 37.29      B
ATOM   2181  N   VAL B 406      62.180  -1.157  51.460  1.00 34.65      B
ATOM   2182  CA  VAL B 406      62.353   0.218  51.027  1.00 35.39      B
ATOM   2183  CB  VAL B 406      63.710   0.421  50.341  1.00 38.27      B
ATOM   2184  CG1 VAL B 406      63.886  -0.606  49.251  1.00 39.50      B
ATOM   2185  CG2 VAL B 406      63.789   1.831  49.759  1.00 38.99      B
ATOM   2186  C   VAL B 406      61.257   0.576  50.041  1.00 34.13      B
ATOM   2187  O   VAL B 406      60.867  -0.250  49.213  1.00 35.33      B
ATOM   2188  N   TYR B 407      60.763   1.806  50.127  1.00 32.42      B
ATOM   2189  CA  TYR B 407      59.694   2.263  49.236  1.00 30.87      B
ATOM   2190  CB  TYR B 407      58.409   2.537  50.032  1.00 30.46      B
ATOM   2191  CG  TYR B 407      57.953   1.435  50.967  1.00 29.77      B
ATOM   2192  CD1 TYR B 407      58.682   1.115  52.121  1.00 27.81      B
ATOM   2193  CE1 TYR B 407      58.269   0.081  52.962  1.00 27.20      B
ATOM   2194  CD2 TYR B 407      56.795   0.695  50.682  1.00 29.18      B
ATOM   2195  CE2 TYR B 407      56.376  -0.335  51.511  1.00 27.89      B
ATOM   2196  CZ  TYR B 407      57.114  -0.645  52.646  1.00 27.80      B
ATOM   2197  OH  TYR B 407      56.711  -1.705  53.430  1.00 26.41      B
ATOM   2198  C   TYR B 407      60.058   3.552  48.507  1.00 29.93      B
ATOM   2199  O   TYR B 407      61.078   4.180  48.790  1.00 30.68      B
ATOM   2200  N   ASP B 408      59.189   3.947  47.583  1.00 29.96      B
ATOM   2201  CA  ASP B 408      59.360   5.181  46.825  1.00 30.52      B
ATOM   2202  CB  ASP B 408      59.226   4.920  45.325  1.00 32.17      B
ATOM   2203  CG  ASP B 408      59.430   6.178  44.504  1.00 35.42      B
ATOM   2204  OD1 ASP B 408      60.450   6.868  44.721  1.00 37.74      B
ATOM   2205  OD2 ASP B 408      58.579   6.483  43.644  1.00 37.68      B
ATOM   2206  C   ASP B 408      58.296   6.195  47.264  1.00 29.92      B
ATOM   2207  O   ASP B 408      57.095   5.995  47.024  1.00 29.81      B
ATOM   2208  N   SER B 409      58.743   7.284  47.895  1.00 28.80      B
ATOM   2209  CA  SER B 409      57.848   8.338  48.400  1.00 28.18      B
ATOM   2210  CB  SER B 409      58.581   9.202  49.442  1.00 25.85      B
ATOM   2211  OG  SER B 409      59.652   9.932  48.869  1.00 23.45      B
```

```
ATOM   2212  C   SER B 409      57.253   9.245  47.320  1.00 29.34      B
ATOM   2213  O   SER B 409      56.259   9.941  47.562  1.00 27.47      B
ATOM   2214  N   ILE B 410      57.861   9.224  46.133  1.00 31.65      B
ATOM   2215  CA  ILE B 410      57.421  10.037  44.994  1.00 34.03      B
ATOM   2216  CB  ILE B 410      58.558  10.242  43.972  1.00 35.56      B
ATOM   2217  CG2 ILE B 410      58.032  11.052  42.783  1.00 34.67      B
ATOM   2218  CG1 ILE B 410      59.747  10.947  44.616  1.00 34.10      B
ATOM   2219  CD1 ILE B 410      60.988  10.910  43.752  1.00 33.88      B
ATOM   2220  C   ILE B 410      56.259   9.409  44.217  1.00 34.05      B
ATOM   2221  O   ILE B 410      55.330  10.101  43.818  1.00 33.24      B
ATOM   2222  N   ASN B 411      56.354   8.107  43.972  1.00 34.44      B
ATOM   2223  CA  ASN B 411      55.327   7.390  43.246  1.00 36.84      B
ATOM   2224  CB  ASN B 411      55.955   6.377  42.273  1.00 39.14      B
ATOM   2225  CG  ASN B 411      56.312   6.993  40.911  1.00 41.27      B
ATOM   2226  OD1 ASN B 411      56.852   8.100  40.834  1.00 41.10      B
ATOM   2227  ND2 ASN B 411      56.017   6.261  39.832  1.00 42.48      B
ATOM   2228  C   ASN B 411      54.428   6.663  44.238  1.00 37.14      B
ATOM   2229  O   ASN B 411      53.466   6.001  43.848  1.00 37.86      B
ATOM   2230  N   LYS B 412      54.748   6.776  45.522  1.00 36.65      B
ATOM   2231  CA  LYS B 412      53.944   6.121  46.546  1.00 35.90      B
ATOM   2232  CB  LYS B 412      52.537   6.742  46.595  1.00 35.46      B
ATOM   2233  CG  LYS B 412      52.373   7.994  47.470  1.00 34.91      B
ATOM   2234  CD  LYS B 412      53.251   9.163  47.023  1.00 33.80      B
ATOM   2235  CE  LYS B 412      52.905  10.407  47.809  1.00 32.17      B
ATOM   2236  NZ  LYS B 412      53.762  11.553  47.463  1.00 32.35      B
ATOM   2237  C   LYS B 412      53.812   4.629  46.256  1.00 35.57      B
ATOM   2238  O   LYS B 412      52.703   4.092  46.252  1.00 35.07      B
ATOM   2239  N   LYS B 413      54.932   3.959  46.007  1.00 35.95      B
ATOM   2240  CA  LYS B 413      54.901   2.523  45.721  1.00 36.16      B
ATOM   2241  CB  LYS B 413      54.977   2.254  44.205  1.00 36.93      B
ATOM   2242  CG  LYS B 413      53.730   2.627  43.387  1.00 40.07      B
ATOM   2243  CD  LYS B 413      53.913   2.308  41.900  1.00 41.03      B
ATOM   2244  CE  LYS B 413      52.629   2.529  41.105  1.00 42.27      B
ATOM   2245  NZ  LYS B 413      51.504   1.699  41.610  1.00 43.62      B
ATOM   2246  C   LYS B 413      56.047   1.798  46.402  1.00 35.81      B
ATOM   2247  O   LYS B 413      57.012   2.417  46.841  1.00 33.26      B
ATOM   2248  N   PHE B 414      55.904   0.481  46.503  1.00 38.03      B
ATOM   2249  CA  PHE B 414      56.909  -0.402  47.090  1.00 39.76      B
ATOM   2250  CB  PHE B 414      56.267  -1.749  47.454  1.00 40.36      B
ATOM   2251  CG  PHE B 414      57.257  -2.806  47.872  1.00 42.43      B
ATOM   2252  CD1 PHE B 414      57.994  -2.667  49.046  1.00 43.87      B
ATOM   2253  CD2 PHE B 414      57.499  -3.914  47.058  1.00 41.81      B
ATOM   2254  CE1 PHE B 414      58.965  -3.614  49.398  1.00 43.95      B
ATOM   2255  CE2 PHE B 414      58.466  -4.863  47.401  1.00 41.35      B
ATOM   2256  CZ  PHE B 414      59.201  -4.712  48.571  1.00 42.36      B
ATOM   2257  C   PHE B 414      57.970  -0.598  46.003  1.00 40.17      B
ATOM   2258  O   PHE B 414      57.642  -0.894  44.854  1.00 39.12      B
ATOM   2259  N   LEU B 415      59.236  -0.425  46.361  1.00 41.37      B
ATOM   2260  CA  LEU B 415      60.305  -0.558  45.386  1.00 42.80      B
ATOM   2261  CB  LEU B 415      61.350   0.539  45.608  1.00 44.70      B
ATOM   2262  CG  LEU B 415      62.211   0.891  44.391  1.00 46.65      B
ATOM   2263  CD1 LEU B 415      61.335   1.453  43.273  1.00 46.10      B
ATOM   2264  CD2 LEU B 415      63.277   1.905  44.794  1.00 47.87      B
ATOM   2265  C   LEU B 415      60.950  -1.941  45.464  1.00 43.04      B
```

ATOM	2266	O	LEU	B	415	60.930	-2.699	44.503	1.00	42.67	B
ATOM	2267	N	LEU	B	416	61.531	-2.288	46.600	1.00	43.99	B
ATOM	2268	CA	LEU	B	416	62.140	-3.607	46.711	1.00	44.67	B
ATOM	2269	CB	LEU	B	416	63.471	-3.667	45.948	1.00	43.56	B
ATOM	2270	CG	LEU	B	416	64.709	-3.198	46.703	1.00	42.12	B
ATOM	2271	CD1	LEU	B	416	65.621	-4.380	46.873	1.00	45.95	B
ATOM	2272	CD2	LEU	B	416	65.421	-2.101	45.951	1.00	41.53	B
ATOM	2273	C	LEU	B	416	62.363	-3.960	48.165	1.00	44.94	B
ATOM	2274	O	LEU	B	416	62.183	-3.123	49.060	1.00	45.50	B
ATOM	2275	N	GLN	B	417	62.747	-5.212	48.393	1.00	45.21	B
ATOM	2276	CA	GLN	B	417	62.999	-5.712	49.744	1.00	45.08	B
ATOM	2277	CB	GLN	B	417	61.984	-6.808	50.120	1.00	43.81	B
ATOM	2278	CG	GLN	B	417	62.106	-7.321	51.555	1.00	40.41	B
ATOM	2279	CD	GLN	B	417	61.077	-8.383	51.890	1.00	39.74	B
ATOM	2280	OE1	GLN	B	417	61.135	-9.507	51.390	1.00	41.92	B
ATOM	2281	NE2	GLN	B	417	60.129	-8.033	52.741	1.00	38.39	B
ATOM	2282	C	GLN	B	417	64.412	-6.279	49.844	1.00	44.86	B
ATOM	2283	O	GLN	B	417	64.906	-6.895	48.897	1.00	43.18	B
ATOM	2284	N	LEU	B	418	65.053	-6.053	50.991	1.00	45.20	B
ATOM	2285	CA	LEU	B	418	66.408	-6.536	51.246	1.00	44.82	B
ATOM	2286	CB	LEU	B	418	67.329	-5.373	51.654	1.00	42.07	B
ATOM	2287	CG	LEU	B	418	67.665	-4.358	50.550	1.00	40.04	B
ATOM	2288	CD1	LEU	B	418	67.984	-2.989	51.123	1.00	38.25	B
ATOM	2289	CD2	LEU	B	418	68.804	-4.885	49.746	1.00	39.20	B
ATOM	2290	C	LEU	B	418	66.337	-7.584	52.357	1.00	46.53	B
ATOM	2291	O	LEU	B	418	65.728	-7.355	53.411	1.00	46.91	B
ATOM	2292	N	SER	B	419	66.929	-8.747	52.086	1.00	47.50	B
ATOM	2293	CA	SER	B	419	66.966	-9.854	53.037	1.00	47.26	B
ATOM	2294	CB	SER	B	419	66.219	-11.066	52.489	1.00	47.58	B
ATOM	2295	OG	SER	B	419	66.861	-11.552	51.330	1.00	47.48	B
ATOM	2296	C	SER	B	419	68.423	-10.219	53.282	1.00	47.06	B
ATOM	2297	O	SER	B	419	69.267	-10.064	52.396	1.00	46.04	B
ATOM	2298	N	GLY	B	420	68.700	-10.697	54.493	1.00	47.22	B
ATOM	2299	CA	GLY	B	420	70.047	-11.059	54.886	1.00	46.53	B
ATOM	2300	C	GLY	B	420	70.121	-11.386	56.366	1.00	47.16	B
ATOM	2301	O	GLY	B	420	70.335	-12.546	56.715	1.00	48.39	B
ATOM	2302	N	HIS	B	421	69.927	-10.390	57.237	1.00	46.12	B
ATOM	2303	CA	HIS	B	421	69.999	-10.611	58.697	1.00	44.26	B
ATOM	2304	CB	HIS	B	421	69.340	-9.451	59.469	1.00	42.53	B
ATOM	2305	CG	HIS	B	421	70.144	-8.187	59.459	1.00	41.48	B
ATOM	2306	CD2	HIS	B	421	70.083	-7.102	58.653	1.00	41.32	B
ATOM	2307	ND1	HIS	B	421	71.231	-7.991	60.282	1.00	41.41	B
ATOM	2308	CE1	HIS	B	421	71.811	-6.845	59.977	1.00	41.09	B
ATOM	2309	NE2	HIS	B	421	71.135	-6.286	58.990	1.00	40.64	B
ATOM	2310	C	HIS	B	421	69.374	-11.937	59.142	1.00	44.07	B
ATOM	2311	O	HIS	B	421	68.254	-12.277	58.746	1.00	43.02	B
ATOM	2312	N	ASP	B	422	70.103	-12.687	59.964	1.00	43.55	B
ATOM	2313	CA	ASP	B	422	69.599	-13.967	60.447	1.00	43.78	B
ATOM	2314	CB	ASP	B	422	70.752	-14.881	60.881	1.00	46.42	B
ATOM	2315	CG	ASP	B	422	71.843	-15.013	59.811	1.00	48.64	B
ATOM	2316	OD1	ASP	B	422	71.518	-15.368	58.649	1.00	47.48	B
ATOM	2317	OD2	ASP	B	422	73.030	-14.762	60.145	1.00	50.00	B
ATOM	2318	C	ASP	B	422	68.634	-13.762	61.609	1.00	42.50	B
ATOM	2319	O	ASP	B	422	67.970	-14.701	62.048	1.00	41.14	B

```
ATOM   2320  N   GLY B 423      68.561 -12.527  62.099  1.00 42.77      B
ATOM   2321  CA  GLY B 423      67.659 -12.192  63.195  1.00 42.60      B
ATOM   2322  C   GLY B 423      66.843 -10.950  62.865  1.00 41.88      B
ATOM   2323  O   GLY B 423      67.107 -10.300  61.855  1.00 42.25      B
ATOM   2324  N   GLY B 424      65.854 -10.615  63.694  1.00 41.87      B
ATOM   2325  CA  GLY B 424      65.036  -9.432  63.433  1.00 41.62      B
ATOM   2326  C   GLY B 424      65.863  -8.158  63.492  1.00 41.35      B
ATOM   2327  O   GLY B 424      66.673  -7.994  64.389  1.00 41.29      B
ATOM   2328  N   VAL B 425      65.682  -7.254  62.541  1.00 41.10      B
ATOM   2329  CA  VAL B 425      66.452  -6.015  62.557  1.00 42.45      B
ATOM   2330  CB  VAL B 425      66.622  -5.464  61.137  1.00 44.73      B
ATOM   2331  CG1 VAL B 425      65.322  -5.641  60.365  1.00 45.42      B
ATOM   2332  CG2 VAL B 425      67.028  -3.987  61.187  1.00 45.68      B
ATOM   2333  C   VAL B 425      65.796  -4.946  63.433  1.00 41.72      B
ATOM   2334  O   VAL B 425      64.600  -4.702  63.318  1.00 42.42      B
ATOM   2335  N   TRP B 426      66.575  -4.305  64.301  1.00 40.55      B
ATOM   2336  CA  TRP B 426      66.016  -3.284  65.177  1.00 39.71      B
ATOM   2337  CB  TRP B 426      66.069  -3.755  66.632  1.00 36.69      B
ATOM   2338  CG  TRP B 426      65.117  -4.874  66.920  1.00 34.11      B
ATOM   2339  CD2 TRP B 426      63.831  -4.774  67.558  1.00 32.48      B
ATOM   2340  CE2 TRP B 426      63.275  -6.072  67.578  1.00 30.88      B
ATOM   2341  CE3 TRP B 426      63.098  -3.715  68.110  1.00 30.22      B
ATOM   2342  CD1 TRP B 426      65.278  -6.185  66.594  1.00 33.27      B
ATOM   2343  NE1 TRP B 426      64.179  -6.910  66.984  1.00 32.30      B
ATOM   2344  CZ2 TRP B 426      62.017  -6.344  68.129  1.00 31.05      B
ATOM   2345  CZ3 TRP B 426      61.845  -3.984  68.661  1.00 30.71      B
ATOM   2346  CH2 TRP B 426      61.319  -5.289  68.666  1.00 30.24      B
ATOM   2347  C   TRP B 426      66.631  -1.889  65.066  1.00 40.31      B
ATOM   2348  O   TRP B 426      66.089  -0.930  65.607  1.00 40.76      B
ATOM   2349  N   ALA B 427      67.759  -1.774  64.379  1.00 41.09      B
ATOM   2350  CA  ALA B 427      68.400  -0.482  64.198  1.00 42.24      B
ATOM   2351  CB  ALA B 427      69.783  -0.481  64.816  1.00 42.58      B
ATOM   2352  C   ALA B 427      68.488  -0.284  62.695  1.00 43.39      B
ATOM   2353  O   ALA B 427      68.658  -1.251  61.952  1.00 44.01      B
ATOM   2354  N   LEU B 428      68.375   0.963  62.248  1.00 44.59      B
ATOM   2355  CA  LEU B 428      68.401   1.261  60.821  1.00 44.89      B
ATOM   2356  CB  LEU B 428      67.015   0.996  60.230  1.00 45.56      B
ATOM   2357  CG  LEU B 428      66.894   0.895  58.717  1.00 46.48      B
ATOM   2358  CD1 LEU B 428      67.730  -0.281  58.221  1.00 47.28      B
ATOM   2359  CD2 LEU B 428      65.434   0.710  58.349  1.00 46.47      B
ATOM   2360  C   LEU B 428      68.761   2.714  60.608  1.00 44.99      B
ATOM   2361  O   LEU B 428      68.132   3.596  61.178  1.00 46.41      B
ATOM   2362  N   LYS B 429      69.766   2.969  59.785  1.00 44.76      B
ATOM   2363  CA  LYS B 429      70.189   4.341  59.519  1.00 44.20      B
ATOM   2364  CB  LYS B 429      71.478   4.631  60.288  1.00 43.86      B
ATOM   2365  CG  LYS B 429      72.022   6.021  60.108  1.00 43.02      B
ATOM   2366  CD  LYS B 429      71.151   7.060  60.779  1.00 40.87      B
ATOM   2367  CE  LYS B 429      71.741   8.447  60.560  1.00 38.32      B
ATOM   2368  NZ  LYS B 429      71.164   9.464  61.464  1.00 34.95      B
ATOM   2369  C   LYS B 429      70.406   4.457  58.021  1.00 44.44      B
ATOM   2370  O   LYS B 429      70.534   3.445  57.344  1.00 44.65      B
ATOM   2371  N   TYR B 430      70.430   5.677  57.496  1.00 45.98      B
ATOM   2372  CA  TYR B 430      70.617   5.884  56.052  1.00 46.60      B
ATOM   2373  CB  TYR B 430      69.403   6.616  55.458  1.00 43.95      B
```

ATOM	2374	CG	TYR	B	430	69.496	6.911	53.973	1.00	41.46	B
ATOM	2375	CD1	TYR	B	430	69.092	5.976	53.027	1.00	40.19	B
ATOM	2376	CE1	TYR	B	430	69.153	6.255	51.664	1.00	38.85	B
ATOM	2377	CD2	TYR	B	430	69.968	8.137	53.520	1.00	40.10	B
ATOM	2378	CE2	TYR	B	430	70.034	8.430	52.164	1.00	39.82	B
ATOM	2379	CZ	TYR	B	430	69.625	7.486	51.232	1.00	39.47	B
ATOM	2380	OH	TYR	B	430	69.691	7.784	49.874	1.00	37.41	B
ATOM	2381	C	TYR	B	430	71.872	6.696	55.767	1.00	47.43	B
ATOM	2382	O	TYR	B	430	72.320	7.476	56.603	1.00	48.99	B
ATOM	2383	N	ALA	B	431	72.439	6.516	54.582	1.00	48.65	B
ATOM	2384	CA	ALA	B	431	73.634	7.263	54.196	1.00	48.95	B
ATOM	2385	CB	ALA	B	431	74.882	6.412	54.420	1.00	49.04	B
ATOM	2386	C	ALA	B	431	73.533	7.683	52.732	1.00	49.00	B
ATOM	2387	O	ALA	B	431	73.298	6.860	51.842	1.00	48.35	B
ATOM	2388	N	HIS	B	432	73.729	8.967	52.482	1.00	49.81	B
ATOM	2389	CA	HIS	B	432	73.627	9.485	51.126	1.00	52.51	B
ATOM	2390	CB	HIS	B	432	74.421	10.787	50.978	1.00	55.86	B
ATOM	2391	CG	HIS	B	432	74.148	11.508	49.695	1.00	60.52	B
ATOM	2392	CD2	HIS	B	432	74.984	12.012	48.757	1.00	62.00	B
ATOM	2393	ND1	HIS	B	432	72.869	11.750	49.238	1.00	62.73	B
ATOM	2394	CE1	HIS	B	432	72.930	12.368	48.072	1.00	63.55	B
ATOM	2395	NE2	HIS	B	432	74.202	12.539	47.757	1.00	63.41	B
ATOM	2396	C	HIS	B	432	74.084	8.497	50.059	1.00	51.80	B
ATOM	2397	O	HIS	B	432	75.031	7.737	50.266	1.00	53.10	B
ATOM	2398	N	GLY	B	433	73.391	8.508	48.923	1.00	50.58	B
ATOM	2399	CA	GLY	B	433	73.741	7.633	47.819	1.00	47.93	B
ATOM	2400	C	GLY	B	433	72.921	6.368	47.714	1.00	47.35	B
ATOM	2401	O	GLY	B	433	73.272	5.462	46.963	1.00	47.94	B
ATOM	2402	N	GLY	B	434	71.823	6.293	48.452	1.00	46.94	B
ATOM	2403	CA	GLY	B	434	71.016	5.090	48.392	1.00	45.51	B
ATOM	2404	C	GLY	B	434	71.722	3.980	49.147	1.00	44.93	B
ATOM	2405	O	GLY	B	434	71.599	2.804	48.824	1.00	45.17	B
ATOM	2406	N	ILE	B	435	72.501	4.353	50.151	1.00	44.36	B
ATOM	2407	CA	ILE	B	435	73.183	3.352	50.943	1.00	43.99	B
ATOM	2408	CB	ILE	B	435	74.701	3.520	50.874	1.00	43.64	B
ATOM	2409	CG2	ILE	B	435	75.375	2.722	51.989	1.00	43.26	B
ATOM	2410	CG1	ILE	B	435	75.196	3.022	49.528	1.00	43.31	B
ATOM	2411	CD1	ILE	B	435	76.656	3.223	49.321	1.00	45.00	B
ATOM	2412	C	ILE	B	435	72.724	3.435	52.395	1.00	44.68	B
ATOM	2413	O	ILE	B	435	72.570	4.518	52.956	1.00	42.73	B
ATOM	2414	N	LEU	B	436	72.486	2.283	53.000	1.00	44.69	B
ATOM	2415	CA	LEU	B	436	72.051	2.273	54.376	1.00	46.18	B
ATOM	2416	CB	LEU	B	436	70.545	2.006	54.468	1.00	46.74	B
ATOM	2417	CG	LEU	B	436	70.020	0.623	54.084	1.00	46.70	B
ATOM	2418	CD1	LEU	B	436	68.660	0.398	54.708	1.00	47.92	B
ATOM	2419	CD2	LEU	B	436	69.953	0.506	52.574	1.00	48.12	B
ATOM	2420	C	LEU	B	436	72.816	1.224	55.176	1.00	47.09	B
ATOM	2421	O	LEU	B	436	73.360	0.268	54.619	1.00	46.99	B
ATOM	2422	N	VAL	B	437	72.862	1.418	56.488	1.00	46.98	B
ATOM	2423	CA	VAL	B	437	73.552	0.497	57.376	1.00	48.04	B
ATOM	2424	CB	VAL	B	437	74.617	1.244	58.228	1.00	49.43	B
ATOM	2425	CG1	VAL	B	437	75.517	0.251	58.948	1.00	48.59	B
ATOM	2426	CG2	VAL	B	437	75.443	2.180	57.333	1.00	49.25	B
ATOM	2427	C	VAL	B	437	72.481	-0.062	58.299	1.00	46.89	B

```
ATOM   2428  O   VAL B 437      71.430   0.551  58.449  1.00 47.34      B
ATOM   2429  N   SER B 438      72.722  -1.222  58.902  1.00 45.63      B
ATOM   2430  CA  SER B 438      71.741  -1.788  59.820  1.00 44.89      B
ATOM   2431  CB  SER B 438      70.729  -2.644  59.072  1.00 44.08      B
ATOM   2432  OG  SER B 438      71.355  -3.758  58.467  1.00 44.83      B
ATOM   2433  C   SER B 438      72.377  -2.622  60.914  1.00 44.82      B
ATOM   2434  O   SER B 438      73.561  -2.949  60.857  1.00 44.21      B
ATOM   2435  N   GLY B 439      71.568  -2.945  61.916  1.00 45.02      B
ATOM   2436  CA  GLY B 439      72.020  -3.751  63.027  1.00 45.90      B
ATOM   2437  C   GLY B 439      70.855  -4.596  63.498  1.00 46.75      B
ATOM   2438  O   GLY B 439      69.809  -4.054  63.843  1.00 45.99      B
ATOM   2439  N   SER B 440      71.006  -5.915  63.496  1.00 49.24      B
ATOM   2440  CA  SER B 440      69.919  -6.773  63.957  1.00 53.65      B
ATOM   2441  CB  SER B 440      69.429  -7.707  62.842  1.00 54.51      B
ATOM   2442  OG  SER B 440      70.342  -8.766  62.610  1.00 56.40      B
ATOM   2443  C   SER B 440      70.368  -7.612  65.146  1.00 54.82      B
ATOM   2444  O   SER B 440      71.474  -7.447  65.660  1.00 54.64      B
ATOM   2445  N   THR B 441      69.490  -8.509  65.576  1.00 57.06      B
ATOM   2446  CA  THR B 441      69.769  -9.392  66.695  1.00 59.13      B
ATOM   2447  CB  THR B 441      68.498 -10.086  67.165  1.00 57.43      B
ATOM   2448  OG1 THR B 441      67.489  -9.101  67.397  1.00 55.10      B
ATOM   2449  CG2 THR B 441      68.761 -10.835  68.455  1.00 59.62      B
ATOM   2450  C   THR B 441      70.778 -10.442  66.262  1.00 61.73      B
ATOM   2451  O   THR B 441      71.212 -11.280  67.048  1.00 62.25      B
ATOM   2452  N   ASP B 442      71.142 -10.379  64.989  1.00 64.11      B
ATOM   2453  CA  ASP B 442      72.098 -11.292  64.403  1.00 65.34      B
ATOM   2454  CB  ASP B 442      72.028 -11.183  62.877  1.00 69.79      B
ATOM   2455  CG  ASP B 442      72.888 -12.220  62.171  1.00 76.04      B
ATOM  -2456  OD1 ASP B 442      72.837 -13.413  62.567  1.00 78.67      B
ATOM   2457  OD2 ASP B 442      73.607 -11.846  61.208  1.00 78.25      B
ATOM   2458  C   ASP B 442      73.490 -10.929  64.903  1.00 64.29      B
ATOM   2459  O   ASP B 442      74.469 -11.621  64.626  1.00 65.24      B
ATOM   2460  N   ARG B 443      73.561  -9.843  65.662  1.00 62.52      B
ATOM   2461  CA  ARG B 443      74.817  -9.346  66.214  1.00 60.60      B
ATOM   2462  CB  ARG B 443      75.495 -10.412  67.088  1.00 61.78      B
ATOM   2463  CG  ARG B 443      74.629 -10.891  68.231  1.00 64.13      B
ATOM   2464  CD  ARG B 443      75.329 -11.918  69.100  1.00 65.45      B
ATOM   2465  NE  ARG B 443      75.805 -13.045  68.312  1.00 68.14      B
ATOM   2466  CZ  ARG B 443      76.062 -14.252  68.804  1.00 69.90      B
ATOM   2467  NH1 ARG B 443      75.885 -14.495  70.096  1.00 69.79      B
ATOM   2468  NH2 ARG B 443      76.493 -15.219  67.998  1.00 70.62      B
ATOM   2469  C   ARG B 443      75.754  -8.904  65.100  1.00 58.12      B
ATOM   2470  O   ARG B 443      76.972  -8.886  65.266  1.00 58.34      B
ATOM   2471  N   THR B 444      75.183  -8.534  63.960  1.00 55.54      B
ATOM   2472  CA  THR B 444      76.005  -8.092  62.841  1.00 53.90      B
ATOM   2473  CB  THR B 444      75.945  -9.106  61.671  1.00 54.03      B
ATOM   2474  OG1 THR B 444      74.590  -9.262  61.232  1.00 53.30      B
ATOM   2475  CG2 THR B 444      76.482 -10.464  62.113  1.00 53.83      B
ATOM   2476  C   THR B 444      75.567  -6.727  62.338  1.00 51.81      B
ATOM   2477  O   THR B 444      74.401  -6.377  62.409  1.00 52.22      B
ATOM   2478  N   VAL B 445      76.510  -5.945  61.846  1.00 49.88      B
ATOM   2479  CA  VAL B 445      76.169  -4.641  61.330  1.00 49.27      B
ATOM   2480  CB  VAL B 445      77.158  -3.569  61.825  1.00 48.34      B
ATOM   2481  CG1 VAL B 445      76.756  -2.196  61.303  1.00 47.11      B
```

```
ATOM   2482  CG2 VAL B 445      77.192  -3.566  63.349  1.00 48.46      B
ATOM   2483  C   VAL B 445      76.233  -4.745  59.813  1.00 50.36      B
ATOM   2484  O   VAL B 445      77.308  -4.656  59.209  1.00 50.35      B
ATOM   2485  N   ARG B 446      75.080  -4.959  59.194  1.00 50.86      B
ATOM   2486  CA  ARG B 446      75.039  -5.081  57.749  1.00 51.42      B
ATOM   2487  CB  ARG B 446      74.024  -6.152  57.329  1.00 52.81      B
ATOM   2488  CG  ARG B 446      74.384  -7.595  57.725  1.00 53.32      B
ATOM   2489  CD  ARG B 446      73.563  -8.565  56.893  1.00 54.70      B
ATOM   2490  NE  ARG B 446      73.801  -9.970  57.206  1.00 55.46      B
ATOM   2491  CZ  ARG B 446      73.462 -10.545  58.353  1.00 57.14      B
ATOM   2492  NH1 ARG B 446      72.878  -9.834  59.303  1.00 59.85      B
ATOM   2493  NH2 ARG B 446      73.677 -11.839  58.548  1.00 57.51      B
ATOM   2494  C   ARG B 446      74.712  -3.759  57.058  1.00 50.94      B
ATOM   2495  O   ARG B 446      73.764  -3.066  57.427  1.00 51.11      B
ATOM   2496  N   VAL B 447      75.525  -3.414  56.063  1.00 49.98      B
ATOM   2497  CA  VAL B 447      75.338  -2.198  55.280  1.00 49.12      B
ATOM   2498  CB  VAL B 447      76.661  -1.360  55.196  1.00 49.77      B
ATOM   2499  CG1 VAL B 447      77.858  -2.268  55.110  1.00 48.80      B
ATOM   2500  CG2 VAL B 447      76.631  -0.433  53.984  1.00 50.29      B
ATOM   2501  C   VAL B 447      74.876  -2.650  53.893  1.00 47.59      B
ATOM   2502  O   VAL B 447      75.433  -3.584  53.334  1.00 46.28      B
ATOM   2503  N   TRP B 448      73.841  -2.001  53.361  1.00 47.07      B
ATOM   2504  CA  TRP B 448      73.278  -2.349  52.058  1.00 46.70      B
ATOM   2505  CB  TRP B 448      71.807  -2.704  52.201  1.00 43.15      B
ATOM   2506  CG  TRP B 448      71.506  -3.423  53.437  1.00 40.87      B
ATOM   2507  CD2 TRP B 448      71.126  -4.793  53.554  1.00 39.93      B
ATOM   2508  CE2 TRP B 448      70.984  -5.067  54.925  1.00 39.42      B
ATOM   2509  CE3 TRP B 448      70.907  -5.820  52.635  1.00 38.21      B
ATOM   2510  CD1 TRP B 448      71.565  -2.930  54.698  1.00 40.70      B
ATOM   2511  NE1 TRP B 448      71.253  -3.910  55.603  1.00 40.18      B
ATOM   2512  CZ2 TRP B 448      70.620  -6.324  55.400  1.00 39.77      B
ATOM   2513  CZ3 TRP B 448      70.547  -7.073  53.110  1.00 38.97      B
ATOM   2514  CH2 TRP B 448      70.413  -7.314  54.480  1.00 38.38      B
ATOM   2515  C   TRP B 448      73.383  -1.223  51.038  1.00 48.93      B
ATOM   2516  O   TRP B 448      73.774  -0.096  51.360  1.00 49.67      B
ATOM   2517  N   ASP B 449      73.001  -1.542  49.803  1.00 51.05      B
ATOM   2518  CA  ASP B 449      73.014  -0.586  48.698  1.00 52.47      B
ATOM   2519  CB  ASP B 449      74.247  -0.830  47.826  1.00 53.58      B
ATOM   2520  CG  ASP B 449      74.259   0.024  46.568  1.00 55.71      B
ATOM   2521  OD1 ASP B 449      73.432  -0.234  45.662  1.00 56.14      B
ATOM   2522  OD2 ASP B 449      75.095   0.954  46.489  1.00 55.67      B
ATOM   2523  C   ASP B 449      71.733  -0.750  47.867  1.00 52.24      B
ATOM   2524  O   ASP B 449      71.541  -1.777  47.225  1.00 52.13      B
ATOM   2525  N   ILE B 450      70.864   0.260  47.883  1.00 52.28      B
ATOM   2526  CA  ILE B 450      69.607   0.199  47.135  1.00 52.23      B
ATOM   2527  CB  ILE B 450      68.729   1.477  47.359  1.00 51.25      B
ATOM   2528  CG2 ILE B 450      67.411   1.352  46.609  1.00 50.40      B
ATOM   2529  CG1 ILE B 450      68.430   1.658  48.851  1.00 50.03      B
ATOM   2530  CD1 ILE B 450      67.617   2.890  49.180  1.00 49.00      B
ATOM   2531  C   ILE B 450      69.849   0.024  45.639  1.00 52.47      B
ATOM   2532  O   ILE B 450      69.266  -0.860  45.024  1.00 52.87      B
ATOM   2533  N   LYS B 451      70.705   0.863  45.060  1.00 53.03      B
ATOM   2534  CA  LYS B 451      71.008   0.779  43.638  1.00 53.15      B
ATOM   2535  CB  LYS B 451      72.346   1.458  43.339  1.00 53.71      B
```

```
ATOM   2536  CG  LYS B 451      72.315   2.978  43.471  0.00 54.77      B
ATOM   2537  CD  LYS B 451      71.228   3.578  42.581  0.00 55.27      B
ATOM   2538  CE  LYS B 451      71.190   5.104  42.643  0.00 55.45      B
ATOM   2539  NZ  LYS B 451      72.286   5.761  41.877  0.00 55.61      B
ATOM   2540  C   LYS B 451      71.059  -0.684  43.212  1.00 53.22      B
ATOM   2541  O   LYS B 451      70.241  -1.139  42.415  1.00 51.85      B
ATOM   2542  N   LYS B 452      72.007  -1.428  43.765  1.00 54.30      B
ATOM   2543  CA  LYS B 452      72.138  -2.833  43.431  1.00 55.55      B
ATOM   2544  CB  LYS B 452      73.549  -3.321  43.756  1.00 56.49      B
ATOM   2545  CG  LYS B 452      74.596  -2.840  42.773  0.00 57.18      B
ATOM   2546  CD  LYS B 452      74.345  -3.420  41.393  0.00 57.78      B
ATOM   2547  CE  LYS B 452      75.353  -2.896  40.391  0.00 58.13      B
ATOM   2548  NZ  LYS B 452      75.066  -3.409  39.027  0.00 58.45      B
ATOM   2549  C   LYS B 452      71.113  -3.701  44.147  1.00 56.44      B
ATOM   2550  O   LYS B 452      70.797  -4.790  43.679  1.00 58.17      B
ATOM   2551  N   GLY B 453      70.594  -3.234  45.279  1.00 56.96      B
ATOM   2552  CA  GLY B 453      69.605  -4.013  46.013  1.00 57.08      B
ATOM   2553  C   GLY B 453      70.167  -5.275  46.650  1.00 57.02      B
ATOM   2554  O   GLY B 453      69.573  -6.353  46.568  1.00 56.26      B
ATOM   2555  N   CYS B 454      71.319  -5.143  47.297  1.00 57.42      B
ATOM   2556  CA  CYS B 454      71.958  -6.281  47.945  1.00 57.82      B
ATOM   2557  CB  CYS B 454      72.844  -7.024  46.937  1.00 59.05      B
ATOM   2558  SG  CYS B 454      74.118  -5.986  46.135  1.00 59.80      B
ATOM   2559  C   CYS B 454      72.800  -5.834  49.136  1.00 57.12      B
ATOM   2560  O   CYS B 454      73.084  -4.644  49.300  1.00 57.22      B
ATOM   2561  N   CYS B 455      73.196  -6.798  49.961  1.00 55.66      B
ATOM   2562  CA  CYS B 455      74.021  -6.529  51.136  1.00 54.95      B
ATOM   2563  CB  CYS B 455      73.831  -7.667  52.140  1.00 54.92      B
ATOM   2564  SG  CYS B 455      74.504  -7.375  53.769  1.00 58.03      B
ATOM   2565  C   CYS B 455      75.485  -6.436  50.678  1.00 54.21      B
ATOM   2566  O   CYS B 455      76.024  -7.404  50.146  1.00 55.39      B
ATOM   2567  N   THR B 456      76.120  -5.277  50.875  1.00 52.48      B
ATOM   2568  CA  THR B 456      77.514  -5.074  50.446  1.00 50.81      B
ATOM   2569  CB  THR B 456      77.771  -3.609  49.987  1.00 50.32      B
ATOM   2570  OG1 THR B 456      77.631  -2.712  51.095  1.00 50.40      B
ATOM   2571  CG2 THR B 456      76.808  -3.217  48.894  1.00 49.71      B
ATOM   2572  C   THR B 456      78.608  -5.434  51.472  1.00 49.16      B
ATOM   2573  O   THR B 456      79.773  -5.613  51.109  1.00 49.26      B
ATOM   2574  N   HIS B 457      78.242  -5.537  52.743  1.00 46.55      B
ATOM   2575  CA  HIS B 457      79.205  -5.871  53.780  1.00 43.83      B
ATOM   2576  CB  HIS B 457      79.956  -4.615  54.229  1.00 43.71      B
ATOM   2577  CG  HIS B 457      80.731  -3.947  53.136  1.00 44.34      B
ATOM   2578  CD2 HIS B 457      80.557  -2.753  52.524  1.00 44.60      B
ATOM   2579  ND1 HIS B 457      81.832  -4.524  52.543  1.00 44.61      B
ATOM   2580  CE1 HIS B 457      82.305  -3.711  51.615  1.00 44.83      B
ATOM   2581  NE2 HIS B 457      81.550  -2.630  51.584  1.00 43.67      B
ATOM   2582  C   HIS B 457      78.512  -6.512  54.979  1.00 42.72      B
ATOM   2583  O   HIS B 457      77.307  -6.342  55.178  1.00 41.66      B
ATOM   2584  N   VAL B 458      79.275  -7.255  55.776  1.00 42.43      B
ATOM   2585  CA  VAL B 458      78.725  -7.918  56.958  1.00 40.96      B
ATOM   2586  CB  VAL B 458      78.386  -9.383  56.655  1.00 41.12      B
ATOM   2587  CG1 VAL B 458      77.331  -9.883  57.628  1.00 39.96      B
ATOM   2588  CG2 VAL B 458      77.913  -9.519  55.225  1.00 40.46      B
ATOM   2589  C   VAL B 458      79.711  -7.852  58.130  1.00 39.97      B
```

```
ATOM   2590  O   VAL B 458      80.391  -8.820  58.456  1.00 38.56      B
ATOM   2591  N   PHE B 459      79.744  -6.690  58.768  1.00 40.60      B
ATOM   2592  CA  PHE B 459      80.623  -6.413  59.892  1.00 41.18      B
ATOM   2593  CB  PHE B 459      80.675  -4.901  60.084  1.00 38.09      B
ATOM   2594  CG  PHE B 459      81.196  -4.158  58.881  1.00 36.10      B
ATOM   2595  CD1 PHE B 459      81.182  -2.765  58.850  1.00 34.95      B
ATOM   2596  CD2 PHE B 459      81.767  -4.847  57.813  1.00 34.29      B
ATOM   2597  CE1 PHE B 459      81.741  -2.055  57.773  1.00 34.55      B
ATOM   2598  CE2 PHE B 459      82.328  -4.160  56.734  1.00 35.73      B
ATOM   2599  CZ  PHE B 459      82.317  -2.755  56.713  1.00 36.03      B
ATOM   2600  C   PHE B 459      80.237  -7.104  61.209  1.00 43.45      B
ATOM   2601  O   PHE B 459      79.357  -6.630  61.921  1.00 44.50      B
ATOM   2602  N   GLU B 460      80.900  -8.216  61.538  1.00 46.24      B
ATOM   2603  CA  GLU B 460      80.608  -8.939  62.783  1.00 47.21      B
ATOM   2604  CB  GLU B 460      80.750 -10.456  62.599  1.00 46.96      B
ATOM   2605  CG  GLU B 460      79.920 -11.030  61.473  1.00 51.03      B
ATOM   2606  CD  GLU B 460      79.971 -12.553  61.386  1.00 52.17      B
ATOM   2607  OE1 GLU B 460      81.079 -13.110  61.261  1.00 54.35      B
ATOM   2608  OE2 GLU B 460      78.897 -13.194  61.428  1.00 51.82      B
ATOM   2609  C   GLU B 460      81.532  -8.491  63.909  1.00 47.31      B
ATOM   2610  O   GLU B 460      82.567  -7.863  63.674  1.00 45.71      B
ATOM   2611  N   GLY B 461      81.147  -8.835  65.134  1.00 48.17      B
ATOM   2612  CA  GLY B 461      81.928  -8.456  66.292  1.00 49.82      B
ATOM   2613  C   GLY B 461      81.102  -8.363  67.561  1.00 50.83      B
ATOM   2614  O   GLY B 461      81.379  -9.074  68.529  1.00 50.20      B
ATOM   2615  N   HIS B 462      80.086  -7.501  67.565  1.00 51.06      B
ATOM   2616  CA  HIS B 462      79.251  -7.346  68.750  1.00 51.73      B
ATOM   2617  CB  HIS B 462      78.010  -6.487  68.443  1.00 50.07      B
ATOM   2618  CG  HIS B 462      78.284  -5.011  68.421  1.00 48.90      B
ATOM   2619  CD2 HIS B 462      78.451  -4.151  67.388  1.00 48.64      B
ATOM   2620  ND1 HIS B 462      78.443  -4.264  69.568  1.00 49.43      B
ATOM   2621  CE1 HIS B 462      78.697  -3.009  69.242  1.00 50.51      B
ATOM   2622  NE2 HIS B 462      78.708  -2.914  67.925  1.00 48.70      B
ATOM   2623  C   HIS B 462      78.846  -8.707  69.315  1.00 52.82      B
ATOM   2624  O   HIS B 462      78.076  -9.459  68.704  1.00 53.62      B
ATOM   2625  N   ASN B 463      79.394  -9.013  70.490  1.00 53.69      B
ATOM   2626  CA  ASN B 463      79.140 -10.269  71.186  1.00 53.67      B
ATOM   2627  CB  ASN B 463      80.119 -10.413  72.369  0.00 53.95      B
ATOM   2628  CG  ASN B 463      81.588 -10.299  71.945  1.00 54.43      B
ATOM   2629  OD1 ASN B 463      82.173 -11.235  71.378  1.00 55.63      B
ATOM   2630  ND2 ASN B 463      82.184  -9.140  72.216  1.00 52.98      B
ATOM   2631  C   ASN B 463      77.699 -10.312  71.686  1.00 53.05      B
ATOM   2632  O   ASN B 463      77.353 -11.133  72.525  1.00 53.74      B
ATOM   2633  N   SER B 464      76.867  -9.414  71.162  1.00 53.52      B
ATOM   2634  CA  SER B 464      75.455  -9.330  71.540  1.00 51.56      B
ATOM   2635  CB  SER B 464      75.324  -8.732  72.946  1.00 52.15      B
ATOM   2636  OG  SER B 464      74.010  -8.925  73.444  1.00 54.03      B
ATOM   2637  C   SER B 464      74.645  -8.487  70.527  1.00 49.85      B
ATOM   2638  O   SER B 464      75.210  -7.852  69.622  1.00 47.81      B
ATOM   2639  N   THR B 465      73.321  -8.496  70.695  1.00 48.25      B
ATOM   2640  CA  THR B 465      72.390  -7.767  69.824  1.00 47.13      B
ATOM   2641  CB  THR B 465      70.924  -7.847  70.344  1.00 48.31      B
ATOM   2642  OG1 THR B 465      70.510  -9.214  70.418  1.00 51.43      B
ATOM   2643  CG2 THR B 465      69.971  -7.098  69.412  1.00 49.57      B
```

```
ATOM   2644  C   THR B 465      72.734  -6.292  69.669  1.00 45.19      B
ATOM   2645  O   THR B 465      73.067  -5.617  70.643  1.00 45.46      B
ATOM   2646  N   VAL B 466      72.636  -5.804  68.433  1.00 42.21      B
ATOM   2647  CA  VAL B 466      72.912  -4.406  68.125  1.00 39.22      B
ATOM   2648  CB  VAL B 466      73.293  -4.241  66.643  1.00 38.21      B
ATOM   2649  CG1 VAL B 466      73.798  -2.829  66.378  1.00 37.18      B
ATOM   2650  CG2 VAL B 466      74.354  -5.264  66.285  1.00 35.99      B
ATOM   2651  C   VAL B 466      71.626  -3.638  68.430  1.00 37.88      B
ATOM   2652  O   VAL B 466      70.655  -3.738  67.691  1.00 35.76      B
ATOM   2653  N   ARG B 467      71.623  -2.886  69.530  1.00 37.28      B
ATOM   2654  CA  ARG B 467      70.440  -2.145  69.938  1.00 36.20      B
ATOM   2655  CB  ARG B 467      70.399  -1.987  71.468  1.00 36.76      B
ATOM   2656  CG  ARG B 467      69.038  -1.513  72.012  1.00 36.98      B
ATOM   2657  CD  ARG B 467      67.945  -2.559  71.762  1.00 39.61      B
ATOM   2658  NE  ARG B 467      66.563  -2.103  71.979  1.00 40.08      B
ATOM   2659  CZ  ARG B 467      65.928  -1.213  71.220  1.00 38.58      B
ATOM   2660  NH1 ARG B 467      66.539  -0.654  70.184  1.00 36.43      B
ATOM   2661  NH2 ARG B 467      64.664  -0.913  71.476  1.00 39.24      B
ATOM   2662  C   ARG B 467      70.314  -0.773  69.283  1.00 35.21      B
ATOM   2663  O   ARG B 467      69.225  -0.213  69.247  1.00 36.67      B
ATOM   2664  N   CYS B 468      71.400  -0.222  68.758  1.00 33.04      B
ATOM   2665  CA  CYS B 468      71.304   1.088  68.127  1.00 33.09      B
ATOM   2666  CB  CYS B 468      71.069   2.167  69.186  1.00 32.72      B
ATOM   2667  SG  CYS B 468      72.414   2.394  70.339  1.00 34.24      B
ATOM   2668  C   CYS B 468      72.533   1.406  67.292  1.00 32.45      B
ATOM   2669  O   CYS B 468      73.473   0.618  67.263  1.00 33.24      B
ATOM   2670  N   LEU B 469      72.522   2.546  66.605  1.00 31.75      B
ATOM   2671  CA  LEU B 469      73.643   2.908  65.747  1.00 32.36      B
ATOM   2672  CB  LEU B 469      73.750   1.917  64.576  1.00 32.24      B
ATOM   2673  CG  LEU B 469      72.822   2.067  63.362  1.00 31.67      B
ATOM   2674  CD1 LEU B 469      73.563   2.673  62.174  1.00 33.01      B
ATOM   2675  CD2 LEU B 469      72.311   0.704  62.982  1.00 33.19      B
ATOM   2676  C   LEU B 469      73.491   4.309  65.179  1.00 32.21      B
ATOM   2677  O   LEU B 469      72.434   4.910  65.285  1.00 32.62      B
ATOM   2678  N   ASP B 470      74.552   4.833  64.581  1.00 33.12      B
ATOM   2679  CA  ASP B 470      74.481   6.149  63.972  1.00 34.33      B
ATOM   2680  CB  ASP B 470      74.431   7.223  65.055  1.00 33.47      B
ATOM   2681  CG  ASP B 470      74.098   8.585  64.501  1.00 32.01      B
ATOM   2682  OD1 ASP B 470      73.302   8.647  63.551  1.00 35.18      B
ATOM   2683  OD2 ASP B 470      74.614   9.589  65.021  1.00 29.33      B
ATOM   2684  C   ASP B 470      75.704   6.330  63.083  1.00 35.86      B
ATOM   2685  O   ASP B 470      76.619   5.509  63.124  1.00 36.56      B
ATOM   2686  N   ILE B 471      75.712   7.384  62.269  1.00 37.44      B
ATOM   2687  CA  ILE B 471      76.841   7.663  61.380  1.00 37.88      B
ATOM   2688  CB  ILE B 471      76.465   7.465  59.889  1.00 36.84      B
ATOM   2689  CG2 ILE B 471      77.698   7.683  59.005  1.00 36.56      B
ATOM   2690  CG1 ILE B 471      75.942   6.050  59.649  1.00 36.63      B
ATOM   2691  CD1 ILE B 471      75.305   5.868  58.283  1.00 35.99      B
ATOM   2692  C   ILE B 471      77.309   9.106  61.569  1.00 38.95      B
ATOM   2693  O   ILE B 471      76.493  10.013  61.769  1.00 39.67      B
ATOM   2694  N   VAL B 472      78.625   9.305  61.522  1.00 39.62      B
ATOM   2695  CA  VAL B 472      79.219  10.631  61.670  1.00 40.41      B
ATOM   2696  CB  VAL B 472      79.932  10.786  63.018  1.00 39.84      B
ATOM   2697  CG1 VAL B 472      78.967  10.468  64.158  1.00 37.97      B
```

```
ATOM   2698  CG2 VAL B 472      81.150   9.862  63.066  1.00 38.84      B
ATOM   2699  C   VAL B 472      80.255  10.802  60.579  1.00 42.22      B
ATOM   2700  O   VAL B 472      80.780   9.820  60.064  1.00 41.41      B
ATOM   2701  N   GLU B 473      80.544  12.048  60.227  1.00 44.76      B
ATOM   2702  CA  GLU B 473      81.539  12.329  59.207  1.00 48.54      B
ATOM   2703  CB  GLU B 473      80.872  12.865  57.934  1.00 49.21      B
ATOM   2704  CG  GLU B 473      81.851  13.193  56.784  1.00 51.32      B
ATOM   2705  CD  GLU B 473      81.143  13.514  55.465  1.00 51.78      B
ATOM   2706  OE1 GLU B 473      80.489  12.609  54.902  1.00 52.52      B
ATOM   2707  OE2 GLU B 473      81.232  14.670  54.996  1.00 52.59      B
ATOM   2708  C   GLU B 473      82.568  13.329  59.737  1.00 50.91      B
ATOM   2709  O   GLU B 473      82.225  14.419  60.205  1.00 50.21      B
ATOM   2710  N   TYR B 474      83.835  12.933  59.683  1.00 53.85      B
ATOM   2711  CA  TYR B 474      84.927  13.775  60.151  1.00 56.31      B
ATOM   2712  CB  TYR B 474      85.504  13.214  61.450  1.00 57.48      B
ATOM   2713  CG  TYR B 474      86.410  14.180  62.164  1.00 59.70      B
ATOM   2714  CD1 TYR B 474      85.925  15.408  62.613  1.00 60.47      B
ATOM   2715  CE1 TYR B 474      86.744  16.305  63.285  1.00 60.97      B
ATOM   2716  CD2 TYR B 474      87.749  13.870  62.402  1.00 60.68      B
ATOM   2717  CE2 TYR B 474      88.581  14.763  63.075  1.00 61.50      B
ATOM   2718  CZ  TYR B 474      88.068  15.978  63.514  1.00 61.92      B
ATOM   2719  OH  TYR B 474      88.875  16.861  64.194  1.00 63.90      B
ATOM   2720  C   TYR B 474      86.001  13.795  59.075  1.00 56.54      B
ATOM   2721  O   TYR B 474      86.293  12.768  58.460  1.00 56.18      B
ATOM   2722  N   LYS B 475      86.589  14.966  58.856  1.00 58.01      B
ATOM   2723  CA  LYS B 475      87.623  15.128  57.840  1.00 59.54      B
ATOM   2724  CB  LYS B 475      88.958  14.579  58.351  1.00 60.12      B
ATOM   2725  CG  LYS B 475      89.453  15.213  59.653  1.00 60.74      B
ATOM   2726  CD  LYS B 475      89.934  16.642  59.449  1.00 61.48      B
ATOM   2727  CE  LYS B 475      90.341  17.283  60.765  0.00 61.92      B
ATOM   2728  NZ  LYS B 475      90.797  18.687  60.568  0.00 62.37      B
ATOM   2729  C   LYS B 475      87.200  14.393  56.563  1.00 60.31      B
ATOM   2730  O   LYS B 475      87.882  13.481  56.093  1.00 61.02      B
ATOM   2731  N   ASN B 476      86.057  14.796  56.020  1.00 60.89      B
ATOM   2732  CA  ASN B 476      85.523  14.199  54.813  1.00 60.87      B
ATOM   2733  CB  ASN B 476      86.260  14.759  53.594  1.00 63.50      B
ATOM   2734  CG  ASN B 476      85.792  16.172  53.224  1.00 66.46      B
ATOM   2735  OD1 ASN B 476      84.649  16.361  52.785  1.00 68.68      B
ATOM   2736  ND2 ASN B 476      86.668  17.167  53.405  1.00 65.78      B
ATOM   2737  C   ASN B 476      85.593  12.676  54.843  1.00 60.30      B
ATOM   2738  O   ASN B 476      85.828  12.036  53.822  1.00 61.52      B
ATOM   2739  N   ILE B 477      85.379  12.095  56.018  1.00 58.81      B
ATOM   2740  CA  ILE B 477      85.395  10.642  56.155  1.00 57.40      B
ATOM   2741  CB  ILE B 477      86.720  10.148  56.780  1.00 58.27      B
ATOM   2742  CG2 ILE B 477      86.741   8.618  56.804  1.00 58.03      B
ATOM   2743  CG1 ILE B 477      87.903  10.659  55.960  0.00 58.14      B
ATOM   2744  CD1 ILE B 477      89.253  10.422  56.599  0.00 58.25      B
ATOM   2745  C   ILE B 477      84.224  10.183  57.030  1.00 55.59      B
ATOM   2746  O   ILE B 477      84.050  10.661  58.151  1.00 55.65      B
ATOM   2747  N   LYS B 478      83.423   9.257  56.515  1.00 52.92      B
ATOM   2748  CA  LYS B 478      82.281   8.760  57.264  1.00 51.69      B
ATOM   2749  CB  LYS B 478      81.106   8.479  56.322  1.00 50.04      B
ATOM   2750  CG  LYS B 478      80.324   9.717  55.899  1.00 47.12      B
ATOM   2751  CD  LYS B 478      78.972   9.329  55.324  1.00 46.70      B
```

```
ATOM   2752  CE  LYS B 478      78.106  10.553  55.048  1.00 45.79      B
ATOM   2753  NZ  LYS B 478      76.681  10.181  54.803  1.00 44.56      B
ATOM   2754  C   LYS B 478      82.591   7.509  58.090  1.00 52.07      B
ATOM   2755  O   LYS B 478      83.279   6.593  57.620  1.00 53.19      B
ATOM   2756  N   TYR B 479      82.076   7.485  59.323  1.00 51.09      B
ATOM   2757  CA  TYR B 479      82.273   6.363  60.250  1.00 49.59      B
ATOM   2758  CB  TYR B 479      83.083   6.815  61.492  1.00 50.00      B
ATOM   2759  CG  TYR B 479      84.438   7.442  61.183  1.00 49.78      B
ATOM   2760  CD1 TYR B 479      84.526   8.594  60.402  1.00 50.71      B
ATOM   2761  CE1 TYR B 479      85.754   9.165  60.062  1.00 49.52      B
ATOM   2762  CD2 TYR B 479      85.629   6.869  61.630  1.00 49.70      B
ATOM   2763  CE2 TYR B 479      86.870   7.438  61.291  1.00 49.93      B
ATOM   2764  CZ  TYR B 479      86.918   8.586  60.502  1.00 49.57      B
ATOM   2765  OH  TYR B 479      88.115   9.155  60.126  1.00 48.42      B
ATOM   2766  C   TYR B 479      80.922   5.790  60.698  1.00 48.39      B
ATOM   2767  O   TYR B 479      79.877   6.381  60.463  1.00 47.95      B
ATOM   2768  N   ILE B 480      80.954   4.629  61.337  1.00 48.14      B
ATOM   2769  CA  ILE B 480      79.742   3.986  61.828  1.00 47.98      B
ATOM   2770  CB  ILE B 480      79.470   2.669  61.090  1.00 47.82      B
ATOM   2771  CG2 ILE B 480      78.250   1.983  61.679  1.00 48.23      B
ATOM   2772  CG1 ILE B 480      79.275   2.929  59.599  1.00 47.92      B
ATOM   2773  CD1 ILE B 480      79.279   1.675  58.768  1.00 46.66      B
ATOM   2774  C   ILE B 480      79.930   3.651  63.308  1.00 48.77      B
ATOM   2775  O   ILE B 480      80.961   3.089  63.699  1.00 49.54      B
ATOM   2776  N   VAL B 481      78.931   3.982  64.124  1.00 48.38      B
ATOM   2777  CA  VAL B 481      78.975   3.718  65.566  1.00 46.50      B
ATOM   2778  CB  VAL B 481      78.917   5.041  66.382  1.00 46.27      B
ATOM   2779  CG1 VAL B 481      79.048   4.749  67.871  1.00 44.39      B
ATOM   2780  CG2 VAL B 481      80.004   5.990  65.914  1.00 45.50      B
ATOM   2781  C   VAL B 481      77.778   2.855  65.962  1.00 45.57      B
ATOM   2782  O   VAL B 481      76.634   3.281  65.823  1.00 45.94      B
ATOM   2783  N   THR B 482      78.039   1.652  66.460  1.00 43.78      B
ATOM   2784  CA  THR B 482      76.963   0.752  66.865  1.00 43.35      B
ATOM   2785  CB  THR B 482      77.050  -0.608  66.091  1.00 44.57      B
ATOM   2786  OG1 THR B 482      78.422  -0.943  65.851  1.00 44.68      B
ATOM   2787  CG2 THR B 482      76.315  -0.523  64.748  1.00 44.18      B
ATOM   2788  C   THR B 482      76.946   0.475  68.379  1.00 42.32      B
ATOM   2789  O   THR B 482      77.979   0.184  68.977  1.00 42.34      B
ATOM   2790  N   GLY B 483      75.769   0.583  68.991  1.00 41.18      B
ATOM   2791  CA  GLY B 483      75.643   0.319  70.410  1.00 42.21      B
ATOM   2792  C   GLY B 483      75.021  -1.057  70.556  1.00 43.25      B
ATOM   2793  O   GLY B 483      74.069  -1.385  69.837  1.00 44.15      B
ATOM   2794  N   SER B 484      75.536  -1.865  71.479  1.00 42.55      B
ATOM   2795  CA  SER B 484      75.018  -3.216  71.650  1.00 42.61      B
ATOM   2796  CB  SER B 484      76.015  -4.236  71.071  1.00 42.00      B
ATOM   2797  OG  SER B 484      75.676  -5.572  71.425  1.00 39.48      B
ATOM   2798  C   SER B 484      74.721  -3.560  73.099  1.00 43.04      B
ATOM   2799  O   SER B 484      75.118  -2.833  74.007  1.00 43.14      B
ATOM   2800  N   ARG B 485      73.993  -4.664  73.294  1.00 43.38      B
ATOM   2801  CA  ARG B 485      73.628  -5.182  74.618  1.00 42.66      B
ATOM   2802  CB  ARG B 485      72.532  -6.233  74.484  1.00 41.35      B
ATOM   2803  CG  ARG B 485      71.309  -5.751  73.737  1.00 41.63      B
ATOM   2804  CD  ARG B 485      70.170  -5.535  74.696  1.00 40.30      B
ATOM   2805  NE  ARG B 485      69.101  -6.499  74.462  1.00 41.39      B
```

```
ATOM   2806  CZ  ARG B 485      67.859  -6.154  74.146  1.00 42.42      B
ATOM   2807  NH1 ARG B 485      67.547  -4.874  74.029  1.00 44.59      B
ATOM   2808  NH2 ARG B 485      66.927  -7.076  73.964  1.00 41.56      B
ATOM   2809  C   ARG B 485      74.879  -5.837  75.200  1.00 43.12      B
ATOM   2810  O   ARG B 485      74.845  -6.448  76.264  1.00 42.36      B
ATOM   2811  N   ASP B 486      75.974  -5.714  74.463  1.00 43.89      B
ATOM   2812  CA  ASP B 486      77.232  -6.263  74.880  1.00 44.86      B
ATOM   2813  CB  ASP B 486      78.100  -6.572  73.646  1.00 45.64      B
ATOM   2814  CG  ASP B 486      78.713  -5.327  73.012  1.00 46.63      B
ATOM   2815  OD1 ASP B 486      78.016  -4.298  72.888  1.00 46.93      B
ATOM   2816  OD2 ASP B 486      79.897  -5.387  72.619  1.00 47.67      B
ATOM   2817  C   ASP B 486      77.887  -5.242  75.807  1.00 45.67      B
ATOM   2818  O   ASP B 486      78.967  -5.486  76.344  1.00 46.05      B
ATOM   2819  N   ASN B 487      77.207  -4.108  76.003  1.00 45.49      B
ATOM   2820  CA  ASN B 487      77.673  -3.017  76.873  1.00 44.88      B
ATOM   2821  CB  ASN B 487      78.223  -3.571  78.188  1.00 44.56      B
ATOM   2822  CG  ASN B 487      77.171  -4.261  79.021  1.00 45.76      B
ATOM   2823  OD1 ASN B 487      76.153  -4.717  78.508  1.00 47.63      B
ATOM   2824  ND2 ASN B 487      77.421  -4.359  80.317  1.00 45.91      B
ATOM   2825  C   ASN B 487      78.748  -2.146  76.242  1.00 44.09      B
ATOM   2826  O   ASN B 487      79.333  -1.306  76.920  1.00 43.58      B
ATOM   2827  N   THR B 488      79.009  -2.347  74.953  1.00 44.03      B
ATOM   2828  CA  THR B 488      80.038  -1.576  74.267  1.00 45.88      B
ATOM   2829  CB  THR B 488      81.264  -2.458  73.895  1.00 46.72      B
ATOM   2830  OG1 THR B 488      81.026  -3.098  72.633  1.00 46.03      B
ATOM   2831  CG2 THR B 488      81.498  -3.545  74.958  1.00 47.35      B
ATOM   2832  C   THR B 488      79.525  -0.958  72.971  1.00 46.36      B
ATOM   2833  O   THR B 488      78.403  -1.224  72.542  1.00 47.28      B
ATOM   2834  N   LEU B 489      80.369  -0.135  72.355  1.00 45.88      B
ATOM   2835  CA  LEU B 489      80.053   0.511  71.090  1.00 46.03      B
ATOM   2836  CB  LEU B 489      79.848   2.015  71.269  1.00 45.02      B
ATOM   2837  CG  LEU B 489      78.651   2.443  72.110  1.00 44.47      B
ATOM   2838  CD1 LEU B 489      79.093   2.732  73.518  1.00 43.21      B
ATOM   2839  CD2 LEU B 489      78.011   3.655  71.484  1.00 45.05      B
ATOM   2840  C   LEU B 489      81.186   0.293  70.102  1.00 47.37      B
ATOM   2841  O   LEU B 489      82.281   0.840  70.280  1.00 48.75      B
ATOM   2842  N   HIS B 490      80.930  -0.507  69.067  1.00 46.28      B
ATOM   2843  CA  HIS B 490      81.940  -0.766  68.040  1.00 44.43      B
ATOM   2844  CB  HIS B 490      81.680  -2.105  67.363  1.00 46.31      B
ATOM   2845  CG  HIS B 490      81.979  -3.288  68.226  1.00 48.42      B
ATOM   2846  CD2 HIS B 490      82.601  -4.456  67.944  1.00 48.94      B
ATOM   2847  ND1 HIS B 490      81.584  -3.371  69.544  1.00 48.72      B
ATOM   2848  CE1 HIS B 490      81.947  -4.542  70.035  1.00 48.74      B
ATOM   2849  NE2 HIS B 490      82.566  -5.220  69.084  1.00 49.32      B
ATOM   2850  C   HIS B 490      81.932   0.332  66.988  1.00 41.63      B
ATOM   2851  O   HIS B 490      80.873   0.804  66.598  1.00 39.88      B
ATOM   2852  N   VAL B 491      83.119   0.727  66.537  1.00 41.79      B
ATOM   2853  CA  VAL B 491      83.268   1.774  65.523  1.00 43.45      B
ATOM   2854  CB  VAL B 491      84.258   2.873  65.987  1.00 43.37      B
ATOM   2855  CG1 VAL B 491      84.565   3.838  64.843  1.00 43.14      B
ATOM   2856  CG2 VAL B 491      83.661   3.642  67.158  1.00 42.84      B
ATOM   2857  C   VAL B 491      83.773   1.199  64.201  1.00 43.94      B
ATOM   2858  O   VAL B 491      84.794   0.515  64.165  1.00 45.06      B
ATOM   2859  N   TRP B 492      83.056   1.479  63.115  1.00 44.26      B
```

```
ATOM   2860  CA  TRP B 492      83.453   0.982  61.804  1.00 43.81      B
ATOM   2861  CB  TRP B 492      82.481  -0.086  61.312  1.00 42.52      B
ATOM   2862  CG  TRP B 492      81.869  -0.922  62.399  1.00 42.97      B
ATOM   2863  CD2 TRP B 492      82.119  -2.308  62.661  1.00 43.02      B
ATOM   2864  CE2 TRP B 492      81.258  -2.696  63.721  1.00 42.64      B
ATOM   2865  CE3 TRP B 492      82.980  -3.262  62.102  1.00 42.84      B
ATOM   2866  CD1 TRP B 492      80.906  -0.535  63.289  1.00 42.27      B
ATOM   2867  NE1 TRP B 492      80.532  -1.593  64.081  1.00 42.22      B
ATOM   2868  CZ2 TRP B 492      81.231  -4.000  64.235  1.00 43.33      B
ATOM   2869  CZ3 TRP B 492      82.955  -4.562  62.613  1.00 43.23      B
ATOM   2870  CH2 TRP B 492      82.083  -4.917  63.670  1.00 43.67      B
ATOM   2871  C   TRP B 492      83.493   2.123  60.804  1.00 44.22      B
ATOM   2872  O   TRP B 492      83.061   3.233  61.094  1.00 43.90      B
ATOM   2873  N   LYS B 493      84.033   1.847  59.627  1.00 45.31      B
ATOM   2874  CA  LYS B 493      84.115   2.855  58.596  1.00 46.28      B
ATOM   2875  CB  LYS B 493      85.515   2.896  57.997  1.00 47.20      B
ATOM   2876  CG  LYS B 493      86.600   3.104  59.021  1.00 48.93      B
ATOM   2877  CD  LYS B 493      87.962   3.179  58.363  0.00 48.94      B
ATOM   2878  CE  LYS B 493      89.061   3.374  59.394  0.00 49.30      B
ATOM   2879  NZ  LYS B 493      90.390   3.550  58.746  0.00 49.52      B
ATOM   2880  C   LYS B 493      83.108   2.522  57.518  1.00 47.32      B
ATOM   2881  O   LYS B 493      82.863   1.349  57.220  1.00 47.63      B
ATOM   2882  N   LEU B 494      82.514   3.563  56.952  1.00 47.99      B
ATOM   2883  CA  LEU B 494      81.539   3.395  55.895  1.00 48.33      B
ATOM   2884  CB  LEU B 494      80.733   4.674  55.717  1.00 48.56      B
ATOM   2885  CG  LEU B 494      79.698   4.594  54.604  1.00 48.11      B
ATOM   2886  CD1 LEU B 494      78.587   3.650  55.032  1.00 47.88      B
ATOM   2887  CD2 LEU B 494      79.156   5.988  54.313  1.00 49.20      B
ATOM   2888  C   LEU B 494      82.298   3.086  54.618  1.00 48.60      B
ATOM   2889  O   LEU B 494      83.009   3.938  54.096  1.00 48.84      B
ATOM   2890  N   PRO B 495      82.170   1.856  54.109  1.00 48.59      B
ATOM   2891  CD  PRO B 495      81.485   0.713  54.729  1.00 48.94      B
ATOM   2892  CA  PRO B 495      82.850   1.438  52.887  1.00 50.38      B
ATOM   2893  CB  PRO B 495      82.345   0.014  52.693  1.00 49.35      B
ATOM   2894  CG  PRO B 495      82.201  -0.461  54.107  1.00 48.48      B
ATOM   2895  C   PRO B 495      82.561   2.342  51.693  1.00 52.37      B
ATOM   2896  O   PRO B 495      81.415   2.741  51.456  1.00 53.23      B
ATOM   2897  N   LYS B 496      83.625   2.669  50.963  1.00 53.80      B
ATOM   2898  CA  LYS B 496      83.557   3.519  49.784  1.00 54.63      B
ATOM   2899  CB  LYS B 496      84.934   4.155  49.529  1.00 55.28      B
ATOM   2900  CG  LYS B 496      86.118   3.196  49.670  1.00 54.90      B
ATOM   2901  CD  LYS B 496      87.443   3.945  49.624  1.00 54.86      B
ATOM   2902  CE  LYS B 496      88.625   3.017  49.840  0.00 55.42      B
ATOM   2903  NZ  LYS B 496      89.917   3.759  49.828  0.00 55.70      B
ATOM   2904  C   LYS B 496      83.100   2.731  48.559  1.00 54.70      B
ATOM   2905  O   LYS B 496      82.693   3.317  47.553  1.00 54.41      B
ATOM   2906  N   ASP B 508      80.076 -10.950  44.143  1.00 87.67      B
ATOM   2907  CA  ASP B 508      81.314 -10.630  44.843  1.00 87.56      B
ATOM   2908  CB  ASP B 508      82.398 -10.224  43.855  1.00 85.57      B
ATOM   2909  CG  ASP B 508      82.370  -8.742  43.565  1.00 84.40      B
ATOM   2910  OD1 ASP B 508      81.334  -8.260  43.072  1.00 83.24      B
ATOM   2911  OD2 ASP B 508      83.371  -8.056  43.855  1.00 83.59      B
ATOM   2912  C   ASP B 508      81.080  -9.451  45.781  1.00 88.88      B
ATOM   2913  O   ASP B 508      82.036  -8.810  46.225  1.00 89.19      B
```

```
ATOM   2914  N   TYR B 509      79.812  -9.155  46.066  1.00 89.80      B
ATOM   2915  CA  TYR B 509      79.455  -8.033  46.939  1.00 89.61      B
ATOM   2916  CB  TYR B 509      78.210  -7.309  46.397  1.00 90.86      B
ATOM   2917  CG  TYR B 509      78.488  -5.981  45.705  1.00 92.99      B
ATOM   2918  CD1 TYR B 509      77.576  -5.455  44.774  1.00 94.09      B
ATOM   2919  CE1 TYR B 509      77.817  -4.236  44.120  1.00 94.93      B
ATOM   2920  CD2 TYR B 509      79.653  -5.252  45.974  1.00 93.03      B
ATOM   2921  CE2 TYR B 509      79.906  -4.032  45.329  1.00 94.38      B
ATOM   2922  CZ  TYR B 509      78.986  -3.530  44.401  1.00 95.32      B
ATOM   2923  OH  TYR B 509      79.241  -2.342  43.743  1.00 95.61      B
ATOM   2924  C   TYR B 509      79.236  -8.425  48.404  1.00 88.37      B
ATOM   2925  O   TYR B 509      79.772  -7.770  49.301  1.00 89.80      B
ATOM   2926  N   PRO B 510      78.448  -9.487  48.672  1.00 86.15      B
ATOM   2927  CD  PRO B 510      77.598 -10.261  47.751  1.00 84.82      B
ATOM   2928  CA  PRO B 510      78.214  -9.897  50.067  1.00 83.98      B
ATOM   2929  CB  PRO B 510      77.276 -11.093  49.923  1.00 84.08      B
ATOM   2930  CG  PRO B 510      76.518 -10.763  48.676  1.00 84.98      B
ATOM   2931  C   PRO B 510      79.508 -10.265  50.800  1.00 81.81      B
ATOM   2932  O   PRO B 510      79.788 -11.441  51.017  1.00 81.76      B
ATOM   2933  N   LEU B 511      80.289  -9.254  51.176  1.00 79.52      B
ATOM   2934  CA  LEU B 511      81.556  -9.462  51.875  1.00 77.45      B
ATOM   2935  CB  LEU B 511      82.466  -8.246  51.701  1.00 75.86      B
ATOM   2936  CG  LEU B 511      82.803  -7.866  50.264  1.00 74.15      B
ATOM   2937  CD1 LEU B 511      83.709  -6.653  50.229  1.00 72.84      B
ATOM   2938  CD2 LEU B 511      83.463  -9.053  49.601  1.00 74.63      B
ATOM   2939  C   LEU B 511      81.323  -9.689  53.355  1.00 77.25      B
ATOM   2940  O   LEU B 511      80.682  -8.878  54.020  1.00 77.95      B
ATOM   2941  N   VAL B 512      81.856 -10.785  53.877  1.00 76.40      B
ATOM   2942  CA  VAL B 512      81.683 -11.100  55.286  1.00 75.66      B
ATOM   2943  CB  VAL B 512      81.075 -12.495  55.458  1.00 74.68      B
ATOM   2944  CG1 VAL B 512      80.748 -12.736  56.917  1.00 73.65      B
ATOM   2945  CG2 VAL B 512      79.843 -12.625  54.587  1.00 73.90      B
ATOM   2946  C   VAL B 512      83.009 -11.040  56.029  1.00 75.90      B
ATOM   2947  O   VAL B 512      84.015 -11.558  55.560  1.00 76.65      B
ATOM   2948  N   PHE B 513      83.007 -10.394  57.187  1.00 75.87      B
ATOM   2949  CA  PHE B 513      84.218 -10.275  57.986  1.00 75.67      B
ATOM   2950  CB  PHE B 513      84.669  -8.820  58.058  1.00 74.40      B
ATOM   2951  CG  PHE B 513      84.758  -8.148  56.722  1.00 74.06      B
ATOM   2952  CD1 PHE B 513      83.611  -7.885  55.981  1.00 74.40      B
ATOM   2953  CD2 PHE B 513      85.987  -7.765  56.208  1.00 74.00      B
ATOM   2954  CE1 PHE B 513      83.686  -7.246  54.752  1.00 74.32      B
ATOM   2955  CE2 PHE B 513      86.077  -7.126  54.979  1.00 73.93      B
ATOM   2956  CZ  PHE B 513      84.921  -6.865  54.249  1.00 74.51      B
ATOM   2957  C   PHE B 513      83.893 -10.780  59.378  1.00 76.17      B
ATOM   2958  O   PHE B 513      83.367 -10.041  60.207  1.00 76.66      B
ATOM   2959  N   HIS B 514      84.203 -12.043  59.631  1.00 76.08      B
ATOM   2960  CA  HIS B 514      83.906 -12.636  60.919  1.00 76.38      B
ATOM   2961  CB  HIS B 514      83.697 -14.139  60.758  1.00 78.44      B
ATOM   2962  CG  HIS B 514      84.803 -14.820  60.022  1.00 81.60      B
ATOM   2963  CD2 HIS B 514      85.579 -15.876  60.360  1.00 82.68      B
ATOM   2964  ND1 HIS B 514      85.232 -14.407  58.780  1.00 82.91      B
ATOM   2965  CE1 HIS B 514      86.228 -15.180  58.384  1.00 84.06      B
ATOM   2966  NE2 HIS B 514      86.458 -16.079  59.324  1.00 83.92      B
ATOM   2967  C   HIS B 514      84.981 -12.355  61.948  1.00 75.65      B
```

```
ATOM   2968  O   HIS B 514      84.997 -12.964  63.016  1.00 75.17      B
ATOM   2969  N   THR B 515      85.880 -11.431  61.632  1.00 75.12      B
ATOM   2970  CA  THR B 515      86.931 -11.076  62.573  1.00 75.68      B
ATOM   2971  CB  THR B 515      88.219 -11.871  62.315  1.00 75.87      B
ATOM   2972  OG1 THR B 515      87.936 -13.276  62.363  1.00 75.87      B
ATOM   2973  CG2 THR B 515      89.255 -11.538  63.375  1.00 74.95      B
ATOM   2974  C   THR B 515      87.245  -9.590  62.492  1.00 75.55      B
ATOM   2975  O   THR B 515      87.642  -9.087  61.445  1.00 75.60      B
ATOM   2976  N   PRO B 516      87.061  -8.869  63.606  1.00 75.61      B
ATOM   2977  CD  PRO B 516      86.520  -9.405  64.867  1.00 76.30      B
ATOM   2978  CA  PRO B 516      87.308  -7.430  63.722  1.00 75.87      B
ATOM   2979  CB  PRO B 516      87.056  -7.161  65.202  1.00 76.07      B
ATOM   2980  CG  PRO B 516      86.008  -8.162  65.550  1.00 76.54      B
ATOM   2981  C   PRO B 516      88.719  -7.025  63.299  1.00 76.37      B
ATOM   2982  O   PRO B 516      88.897  -6.183  62.415  1.00 75.84      B
ATOM   2983  N   GLU B 517      89.714  -7.626  63.949  1.00 76.93      B
ATOM   2984  CA  GLU B 517      91.126  -7.356  63.676  1.00 76.76      B
ATOM   2985  CB  GLU B 517      91.996  -8.320  64.492  1.00 78.63      B
ATOM   2986  CG  GLU B 517      93.496  -8.083  64.384  1.00 81.28      B
ATOM   2987  CD  GLU B 517      93.944  -6.839  65.123  1.00 82.27      B
ATOM   2988  OE1 GLU B 517      95.171  -6.593  65.192  1.00 83.01      B
ATOM   2989  OE2 GLU B 517      93.066  -6.107  65.630  1.00 82.62      B
ATOM   2990  C   GLU B 517      91.448  -7.505  62.189  1.00 75.46      B
ATOM   2991  O   GLU B 517      92.318  -6.812  61.663  1.00 75.08      B
ATOM   2992  N   GLU B 518      90.733  -8.411  61.525  1.00 73.54      B
ATOM   2993  CA  GLU B 518      90.927  -8.681  60.106  1.00 71.48      B
ATOM   2994  CB  GLU B 518      90.530 -10.124  59.793  0.00 72.44      B
ATOM   2995  CG  GLU B 518      90.797 -10.526  58.359  0.00 73.10      B
ATOM   2996  CD  GLU B 518      90.441 -11.970  58.079  0.00 73.51      B
ATOM   2997  OE1 GLU B 518      89.258 -12.335  58.243  0.00 73.72      B
ATOM   2998  OE2 GLU B 518      91.346 -12.741  57.695  0.00 73.72      B
ATOM   2999  C   GLU B 518      90.145  -7.730  59.199  1.00 70.28      B
ATOM   3000  O   GLU B 518      90.596  -7.400  58.098  1.00 69.72      B
ATOM   3001  N   ASN B 519      88.977  -7.296  59.676  1.00 68.04      B
ATOM   3002  CA  ASN B 519      88.087  -6.380  58.947  1.00 65.05      B
ATOM   3003  CB  ASN B 519      86.773  -6.224  59.718  1.00 63.79      B
ATOM   3004  CG  ASN B 519      85.805  -5.267  59.053  1.00 62.26      B
ATOM   3005  OD1 ASN B 519      84.702  -5.066  59.548  1.00 62.79      B
ATOM   3006  ND2 ASN B 519      86.204  -4.676  57.933  1.00 60.05      B
ATOM   3007  C   ASN B 519      88.716  -5.000  58.728  1.00 63.93      B
ATOM   3008  O   ASN B 519      88.842  -4.220  59.669  1.00 64.23      B
ATOM   3009  N   PRO B 520      89.090  -4.673  57.473  1.00 62.40      B
ATOM   3010  CD  PRO B 520      88.866  -5.499  56.274  1.00 61.90      B
ATOM   3011  CA  PRO B 520      89.711  -3.396  57.096  1.00 60.68      B
ATOM   3012  CB  PRO B 520      89.820  -3.497  55.577  1.00 60.59      B
ATOM   3013  CG  PRO B 520      89.895  -4.957  55.331  1.00 61.94      B
ATOM   3014  C   PRO B 520      88.906  -2.174  57.500  1.00 60.35      B
ATOM   3015  O   PRO B 520      89.403  -1.049  57.445  1.00 60.91      B
ATOM   3016  N   TYR B 521      87.657  -2.399  57.888  1.00 58.53      B
ATOM   3017  CA  TYR B 521      86.774  -1.314  58.276  1.00 56.62      B
ATOM   3018  CB  TYR B 521      85.410  -1.538  57.636  1.00 56.52      B
ATOM   3019  CG  TYR B 521      85.470  -1.631  56.133  1.00 55.43      B
ATOM   3020  CD1 TYR B 521      85.625  -0.493  55.356  1.00 53.35      B
ATOM   3021  CE1 TYR B 521      85.684  -0.568  53.980  1.00 52.25      B
```

```
ATOM   3022  CD2 TYR B 521      85.378  -2.860  55.487  1.00 55.47      B
ATOM   3023  CE2 TYR B 521      85.437  -2.946  54.109  1.00 54.04      B
ATOM   3024  CZ  TYR B 521      85.587  -1.792  53.360  1.00 53.20      B
ATOM   3025  OH  TYR B 521      85.611  -1.862  51.986  1.00 53.19      B
ATOM   3026  C   TYR B 521      86.618  -1.168  59.782  1.00 56.07      B
ATOM   3027  O   TYR B 521      86.225  -0.109  60.264  1.00 55.68      B
ATOM   3028  N   PHE B 522      86.929  -2.227  60.521  1.00 55.73      B
ATOM   3029  CA  PHE B 522      86.797  -2.207  61.969  1.00 55.79      B
ATOM   3030  CB  PHE B 522      86.993  -3.605  62.543  1.00 57.01      B
ATOM   3031  CG  PHE B 522      86.935  -3.654  64.046  1.00 59.45      B
ATOM   3032  CD1 PHE B 522      85.730  -3.458  64.719  1.00 60.43      B
ATOM   3033  CD2 PHE B 522      88.084  -3.895  64.794  1.00 59.23      B
ATOM   3034  CE1 PHE B 522      85.672  -3.505  66.119  1.00 60.50      B
ATOM   3035  CE2 PHE B 522      88.032  -3.943  66.192  1.00 59.21      B
ATOM   3036  CZ  PHE B 522      86.825  -3.749  66.856  1.00 58.74      B
ATOM   3037  C   PHE B 522      87.764  -1.267  62.668  1.00 55.79      B
ATOM   3038  O   PHE B 522      88.899  -1.643  62.962  1.00 56.44      B
ATOM   3039  N   VAL B 523      87.314  -0.048  62.951  1.00 56.06      B
ATOM   3040  CA  VAL B 523      88.155   0.924  63.650  1.00 55.15      B
ATOM   3041  CB  VAL B 523      87.445   2.271  63.817  1.00 53.14      B
ATOM   3042  CG1 VAL B 523      88.324   3.223  64.601  1.00 51.48      B
ATOM   3043  CG2 VAL B 523      87.113   2.844  62.460  1.00 53.68      B
ATOM   3044  C   VAL B 523      88.506   0.384  65.035  1.00 55.15      B
ATOM   3045  O   VAL B 523      89.675   0.140  65.331  1.00 55.89      B
ATOM   3046  N   GLY B 524      87.489   0.187  65.870  1.00 53.67      B
ATOM   3047  CA  GLY B 524      87.726  -0.325  67.205  1.00 52.15      B
ATOM   3048  C   GLY B 524      86.521  -0.286  68.127  1.00 50.48      B
ATOM   3049  O   GLY B 524      85.504   0.329  67.821  1.00 50.52      B
ATOM   3050  N   VAL B 525      86.643  -0.933  69.277  1.00 48.79      B
ATOM   3051  CA  VAL B 525      85.555  -0.975  70.232  1.00 48.07      B
ATOM   3052  CB  VAL B 525      85.354  -2.418  70.744  1.00 46.89      B
ATOM   3053  CG1 VAL B 525      86.674  -3.138  70.750  1.00 45.99      B
ATOM   3054  CG2 VAL B 525      84.732  -2.403  72.130  1.00 45.90      B
ATOM   3055  C   VAL B 525      85.800  -0.015  71.392  1.00 47.57      B
ATOM   3056  O   VAL B 525      86.938   0.175  71.805  1.00 46.79      B
ATOM   3057  N   LEU B 526      84.727   0.603  71.894  1.00 48.52      B
ATOM   3058  CA  LEU B 526      84.811   1.567  73.005  1.00 48.97      B
ATOM   3059  CB  LEU B 526      84.199   2.910  72.583  1.00 47.57      B
ATOM   3060  CG  LEU B 526      84.696   3.601  71.310  1.00 47.85      B
ATOM   3061  CD1 LEU B 526      83.713   4.694  70.936  1.00 48.90      B
ATOM   3062  CD2 LEU B 526      86.082   4.170  71.496  1.00 46.34      B
ATOM   3063  C   LEU B 526      84.078   1.047  74.257  1.00 49.07      B
ATOM   3064  O   LEU B 526      82.862   1.207  74.382  1.00 49.55      B
ATOM   3065  N   ARG B 527      84.820   0.425  75.174  1.00 48.77      B
ATOM   3066  CA  ARG B 527      84.239  -0.119  76.402  1.00 48.18      B
ATOM   3067  CB  ARG B 527      85.016  -1.349  76.877  1.00 47.43      B
ATOM   3068  CG  ARG B 527      84.725  -2.604  76.074  1.00 47.62      B
ATOM   3069  CD  ARG B 527      85.540  -3.794  76.557  1.00 45.88      B
ATOM   3070  NE  ARG B 527      86.528  -4.196  75.561  1.00 44.94      B
ATOM   3071  CZ  ARG B 527      86.259  -4.860  74.439  1.00 43.61      B
ATOM   3072  NH1 ARG B 527      85.014  -5.218  74.152  1.00 41.64      B
ATOM   3073  NH2 ARG B 527      87.246  -5.158  73.594  1.00 41.55      B
ATOM   3074  C   ARG B 527      84.214   0.907  77.515  1.00 47.73      B
ATOM   3075  O   ARG B 527      85.162   1.662  77.703  1.00 46.73      B
```

ATOM	3076	N	GLY	B	528	83.120	0.929	78.259	1.00	48.05	B
ATOM	3077	CA	GLY	B	528	83.013	1.888	79.338	1.00	49.61	B
ATOM	3078	C	GLY	B	528	81.677	1.823	80.047	1.00	50.20	B
ATOM	3079	O	GLY	B	528	81.510	2.397	81.120	1.00	50.44	B
ATOM	3080	N	HIS	B	529	80.718	1.126	79.448	1.00	51.40	B
ATOM	3081	CA	HIS	B	529	79.392	0.990	80.040	1.00	52.69	B
ATOM	3082	CB	HIS	B	529	78.308	1.270	78.997	1.00	53.42	B
ATOM	3083	CG	HIS	B	529	77.908	2.711	78.931	1.00	54.66	B
ATOM	3084	CD2	HIS	B	529	78.036	3.710	79.836	1.00	54.96	B
ATOM	3085	ND1	HIS	B	529	77.284	3.264	77.835	1.00	54.53	B
ATOM	3086	CE1	HIS	B	529	77.046	4.542	78.066	1.00	54.69	B
ATOM	3087	NE2	HIS	B	529	77.493	4.837	79.273	1.00	55.98	B
ATOM	3088	C	HIS	B	529	79.174	-0.376	80.664	1.00	52.47	B
ATOM	3089	O	HIS	B	529	79.576	-1.396	80.112	1.00	53.72	B
ATOM	3090	N	MSE	B	530	78.531	-0.379	81.825	1.00	52.35	B
ATOM	3091	CA	MSE	B	530	78.260	-1.603	82.568	1.00	51.79	B
ATOM	3092	CB	MSE	B	530	78.325	-1.325	84.068	1.00	54.89	B
ATOM	3093	CG	MSE	B	530	79.640	-0.727	84.520	1.00	59.05	B
ATOM	3094	SE	MSE	B	530	81.160	-1.831	84.066	1.00	66.13	B
ATOM	3095	CE	MSE	B	530	81.008	-3.077	85.560	1.00	62.20	B
ATOM	3096	C	MSE	B	530	76.894	-2.153	82.241	1.00	50.13	B
ATOM	3097	O	MSE	B	530	76.318	-2.887	83.036	1.00	49.11	B
ATOM	3098	N	ALA	B	531	76.379	-1.800	81.070	1.00	49.94	B
ATOM	3099	CA	ALA	B	531	75.055	-2.246	80.658	1.00	48.69	B
ATOM	3100	CB	ALA	B	531	73.999	-1.553	81.498	1.00	48.43	B
ATOM	3101	C	ALA	B	531	74.843	-1.928	79.189	1.00	47.77	B
ATOM	3102	O	ALA	B	531	75.669	-1.256	78.566	1.00	48.05	B
ATOM	3103	N	SER	B	532	73.731	-2.414	78.645	1.00	46.82	B
ATOM	3104	CA	SER	B	532	73.380	-2.196	77.242	1.00	45.70	B
ATOM	3105	CB	SER	B	532	72.036	-2.855	76.921	1.00	45.79	B
ATOM	3106	OG	SER	B	532	71.413	-2.223	75.811	1.00	44.70	B
ATOM	3107	C	SER	B	532	73.306	-0.733	76.839	1.00	44.93	B
ATOM	3108	O	SER	B	532	72.834	0.118	77.595	1.00	45.32	B
ATOM	3109	N	VAL	B	533	73.775	-0.469	75.627	1.00	43.79	B
ATOM	3110	CA	VAL	B	533	73.771	0.865	75.038	1.00	43.92	B
ATOM	3111	CB	VAL	B	533	75.002	1.045	74.123	1.00	42.68	B
ATOM	3112	CG1	VAL	B	533	74.893	2.335	73.336	1.00	42.48	B
ATOM	3113	CG2	VAL	B	533	76.274	1.027	74.965	1.00	41.21	B
ATOM	3114	C	VAL	B	533	72.480	1.013	74.215	1.00	43.88	B
ATOM	3115	O	VAL	B	533	72.398	0.518	73.085	1.00	43.85	B
ATOM	3116	N	ARG	B	534	71.479	1.689	74.787	1.00	42.61	B
ATOM	3117	CA	ARG	B	534	70.174	1.867	74.136	1.00	40.98	B
ATOM	3118	CB	ARG	B	534	69.074	2.081	75.177	1.00	41.23	B
ATOM	3119	CG	ARG	B	534	67.896	1.146	75.017	1.00	42.21	B
ATOM	3120	CD	ARG	B	534	66.586	1.862	74.752	1.00	43.49	B
ATOM	3121	NE	ARG	B	534	66.301	2.077	73.331	1.00	45.72	B
ATOM	3122	CZ	ARG	B	534	65.097	1.903	72.792	1.00	47.54	B
ATOM	3123	NH1	ARG	B	534	64.093	1.508	73.563	1.00	46.82	B
ATOM	3124	NH2	ARG	B	534	64.884	2.136	71.499	1.00	50.38	B
ATOM	3125	C	ARG	B	534	70.104	3.015	73.162	1.00	39.36	B
ATOM	3126	O	ARG	B	534	69.339	2.975	72.200	1.00	38.05	B
ATOM	3127	N	THR	B	535	70.889	4.050	73.426	1.00	38.74	B
ATOM	3128	CA	THR	B	535	70.869	5.217	72.566	1.00	38.25	B
ATOM	3129	CB	THR	B	535	70.062	6.362	73.233	1.00	39.86	B

```
ATOM   3130  OG1 THR B 535      70.130   7.534  72.411  1.00 42.15      B
ATOM   3131  CG2 THR B 535      70.596   6.661  74.630  1.00 39.79      B
ATOM   3132  C   THR B 535      72.263   5.686  72.189  1.00 36.40      B
ATOM   3133  O   THR B 535      73.212   5.478  72.934  1.00 34.48      B
ATOM   3134  N   VAL B 536      72.369   6.300  71.013  1.00 36.97      B
ATOM   3135  CA  VAL B 536      73.637   6.798  70.482  1.00 38.48      B
ATOM   3136  CB  VAL B 536      74.365   5.725  69.663  1.00 39.79      B
ATOM   3137  CG1 VAL B 536      75.570   6.344  68.958  1.00 39.98      B
ATOM   3138  CG2 VAL B 536      74.807   4.588  70.561  1.00 42.70      B
ATOM   3139  C   VAL B 536      73.417   7.969  69.538  1.00 37.98      B
ATOM   3140  O   VAL B 536      72.705   7.836  68.544  1.00 39.94      B
ATOM   3141  N   SER B 537      74.037   9.105  69.832  1.00 36.75      B
ATOM   3142  CA  SER B 537      73.904  10.281  68.978  1.00 35.47      B
ATOM   3143  CB  SER B 537      72.974  11.296  69.646  1.00 36.17      B
ATOM   3144  OG  SER B 537      73.057  12.572  69.032  1.00 36.43      B
ATOM   3145  C   SER B 537      75.280  10.889  68.744  1.00 34.85      B
ATOM   3146  O   SER B 537      76.071  11.009  69.671  1.00 33.64      B
ATOM   3147  N   GLY B 538      75.575  11.258  67.507  1.00 34.65      B
ATOM   3148  CA  GLY B 538      76.875  11.836  67.243  1.00 37.80      B
ATOM   3149  C   GLY B 538      76.900  12.740  66.030  1.00 39.65      B
ATOM   3150  O   GLY B 538      75.937  12.783  65.270  1.00 39.10      B
ATOM   3151  N   HIS B 539      78.004  13.462  65.857  1.00 42.51      B
ATOM   3152  CA  HIS B 539      78.193  14.382  64.736  1.00 44.95      B
ATOM   3153  CB  HIS B 539      77.370  15.657  64.927  1.00 48.76      B
ATOM   3154  CG  HIS B 539      75.912  15.402  65.134  1.00 54.64      B
ATOM   3155  CD2 HIS B 539      75.121  15.566  66.221  1.00 55.81      B
ATOM   3156  ND1 HIS B 539      75.112  14.845  64.158  1.00 55.89      B
ATOM   3157  CE1 HIS B 539      73.891  14.677  64.635  1.00 56.19      B
ATOM   3158  NE2 HIS B 539      73.870  15.106  65.885  1.00 56.92      B
ATOM   3159  C   HIS B 539      79.665  14.753  64.709  1.00 45.08      B
ATOM   3160  O   HIS B 539      80.167  15.351  65.659  1.00 45.61      B
ATOM   3161  N   GLY B 540      80.357  14.409  63.627  1.00 44.60      B
ATOM   3162  CA  GLY B 540      81.773  14.727  63.538  1.00 44.51      B
ATOM   3163  C   GLY B 540      82.612  13.714  64.300  1.00 44.45      B
ATOM   3164  O   GLY B 540      82.356  12.519  64.188  1.00 44.43      B
ATOM   3165  N   ASN B 541      83.612  14.182  65.054  1.00 44.24      B
ATOM   3166  CA  ASN B 541      84.482  13.304  65.841  1.00 43.77      B
ATOM   3167  CB  ASN B 541      85.914  13.855  65.925  1.00 43.91      B
ATOM   3168  CG  ASN B 541      86.011  15.119  66.773  1.00 45.62      B
ATOM   3169  OD1 ASN B 541      85.399  16.139  66.449  1.00 46.42      B
ATOM   3170  ND2 ASN B 541      86.783  15.054  67.867  1.00 45.00      B
ATOM   3171  C   ASN B 541      83.949  13.134  67.257  1.00 43.38      B
ATOM   3172  O   ASN B 541      84.662  12.651  68.139  1.00 44.20      B
ATOM   3173  N   ILE B 542      82.697  13.530  67.475  1.00 41.65      B
ATOM   3174  CA  ILE B 542      82.067  13.418  68.789  1.00 40.51      B
ATOM   3175  CB  ILE B 542      81.681  14.821  69.350  1.00 41.10      B
ATOM   3176  CG2 ILE B 542      81.158  14.690  70.779  1.00 39.51      B
ATOM   3177  CG1 ILE B 542      82.893  15.753  69.325  1.00 39.00      B
ATOM   3178  CD1 ILE B 542      84.043  15.278  70.192  1.00 38.09      B
ATOM   3179  C   ILE B 542      80.795  12.560  68.744  1.00 39.78      B
ATOM   3180  O   ILE B 542      79.939  12.740  67.870  1.00 38.52      B
ATOM   3181  N   VAL B 543      80.687  11.630  69.691  1.00 38.75      B
ATOM   3182  CA  VAL B 543      79.523  10.752  69.799  1.00 38.25      B
ATOM   3183  CB  VAL B 543      79.775   9.342  69.183  1.00 37.58      B
```

```
ATOM   3184  CG1 VAL B 543      78.596   8.430  69.454  1.00 34.60      B
ATOM   3185  CG2 VAL B 543      79.995   9.459  67.678  1.00 39.64      B
ATOM   3186  C   VAL B 543      79.198  10.573  71.270  1.00 37.91      B
ATOM   3187  O   VAL B 543      80.098  10.411  72.091  1.00 40.30      B
ATOM   3188  N   VAL B 544      77.913  10.602  71.605  1.00 35.82      B
ATOM   3189  CA  VAL B 544      77.490  10.435  72.985  1.00 32.38      B
ATOM   3190  CB  VAL B 544      76.637  11.600  73.437  1.00 31.34      B
ATOM   3191  CG1 VAL B 544      76.364  11.471  74.913  1.00 31.93      B
ATOM   3192  CG2 VAL B 544      77.321  12.904  73.104  1.00 30.92      B
ATOM   3193  C   VAL B 544      76.652   9.186  73.089  1.00 31.39      B
ATOM   3194  O   VAL B 544      75.764   8.976  72.279  1.00 32.39      B
ATOM   3195  N   SER B 545      76.913   8.359  74.089  1.00 31.37      B
ATOM   3196  CA  SER B 545      76.136   7.135  74.238  1.00 32.82      B
ATOM   3197  CB  SER B 545      77.067   5.911  74.166  1.00 33.04      B
ATOM   3198  OG  SER B 545      77.887   5.768  75.328  1.00 31.94      B
ATOM   3199  C   SER B 545      75.290   7.062  75.522  1.00 34.31      B
ATOM   3200  O   SER B 545      75.663   7.595  76.576  1.00 35.23      B
ATOM   3201  N   GLY B 546      74.157   6.373  75.421  1.00 35.10      B
ATOM   3202  CA  GLY B 546      73.271   6.209  76.558  1.00 35.16      B
ATOM   3203  C   GLY B 546      73.064   4.744  76.889  1.00 35.12      B
ATOM   3204  O   GLY B 546      72.627   3.952  76.048  1.00 36.06      B
ATOM   3205  N   SER B 547      73.370   4.377  78.122  1.00 34.92      B
ATOM   3206  CA  SER B 547      73.219   2.996  78.520  1.00 35.83      B
ATOM   3207  CB  SER B 547      74.542   2.450  79.054  1.00 36.42      B
ATOM   3208  OG  SER B 547      74.376   1.145  79.580  1.00 37.41      B
ATOM   3209  C   SER B 547      72.146   2.811  79.569  1.00 36.27      B
ATOM   3210  O   SER B 547      71.561   3.776  80.043  1.00 35.05      B
ATOM   3211  N   TYR B 548      71.881   1.555  79.908  1.00 38.32      B
ATOM   3212  CA  TYR B 548      70.890   1.227  80.916  1.00 40.30      B
ATOM   3213  CB  TYR B 548      70.288  -0.146  80.629  1.00 42.68      B
ATOM   3214  CG  TYR B 548      69.117  -0.134  79.670  1.00 45.80      B
ATOM   3215  CD1 TYR B 548      68.593   1.068  79.174  1.00 47.24      B
ATOM   3216  CE1 TYR B 548      67.472   1.074  78.345  1.00 47.96      B
ATOM   3217  CD2 TYR B 548      68.494  -1.322  79.302  1.00 45.36      B
ATOM   3218  CE2 TYR B 548      67.385  -1.325  78.481  1.00 46.33      B
ATOM   3219  CZ  TYR B 548      66.873  -0.135  78.008  1.00 47.54      B
ATOM   3220  OH  TYR B 548      65.744  -0.162  77.223  1.00 49.19      B
ATOM   3221  C   TYR B 548      71.550   1.228  82.289  1.00 40.55      B
ATOM   3222  O   TYR B 548      70.898   0.990  83.305  1.00 40.82      B
ATOM   3223  N   ASP B 549      72.852   1.496  82.315  1.00 40.33      B
ATOM   3224  CA  ASP B 549      73.574   1.523  83.572  1.00 40.21      B
ATOM   3225  CB  ASP B 549      75.053   1.177  83.352  1.00 38.64      B
ATOM   3226  CG  ASP B 549      75.813   2.287  82.659  1.00 39.21      B
ATOM   3227  OD1 ASP B 549      75.195   3.348  82.399  1.00 39.42      B
ATOM   3228  OD2 ASP B 549      77.025   2.106  82.389  1.00 35.60      B
ATOM   3229  C   ASP B 549      73.437   2.905  84.207  1.00 41.08      B
ATOM   3230  O   ASP B 549      74.180   3.251  85.125  1.00 41.91      B
ATOM   3231  N   ASN B 550      72.490   3.693  83.696  1.00 41.46      B
ATOM   3232  CA  ASN B 550      72.213   5.043  84.208  1.00 41.90      B
ATOM   3233  CB  ASN B 550      71.853   4.982  85.696  1.00 42.29      B
ATOM   3234  CG  ASN B 550      70.885   3.882  86.013  1.00 42.40      B
ATOM   3235  OD1 ASN B 550      70.421   3.181  85.117  1.00 44.98      B
ATOM   3236  ND2 ASN B 550      70.563   3.723  87.289  1.00 41.54      B
ATOM   3237  C   ASN B 550      73.430   5.944  84.049  1.00 41.35      B
```

	ATOM	3238	O	ASN	B	550	73.934	6.498	85.034	1.00	41.70	B
	ATOM	3239	N	THR	B	551	73.891	6.101	82.816	1.00	40.29	B
	ATOM	3240	CA	THR	B	551	75.081	6.890	82.562	1.00	40.46	B
	ATOM	3241	CB	THR	B	551	76.344	6.109	83.031	1.00	40.37	B
5	ATOM	3242	OG1	THR	B	551	76.524	6.278	84.437	1.00	40.39	B
	ATOM	3243	CG2	THR	B	551	77.576	6.547	82.288	1.00	39.19	B
	ATOM	3244	C	THR	B	551	75.230	7.167	81.080	1.00	41.05	B
	ATOM	3245	O	THR	B	551	74.793	6.374	80.250	1.00	41.68	B
	ATOM	3246	N	LEU	B	552	75.849	8.295	80.754	1.00	40.71	B
10	ATOM	3247	CA	LEU	B	552	76.098	8.659	79.368	1.00	40.16	B
	ATOM	3248	CB	LEU	B	552	75.354	9.943	78.994	1.00	39.03	B
	ATOM	3249	CG	LEU	B	552	73.828	9.882	78.968	1.00	38.53	B
	ATOM	3250	CD1	LEU	B	552	73.257	10.693	80.130	1.00	38.23	B
	ATOM	3251	CD2	LEU	B	552	73.327	10.416	77.631	1.00	37.33	B
15	ATOM	3252	C	LEU	B	552	77.591	8.888	79.253	1.00	40.99	B
	ATOM	3253	O	LEU	B	552	78.225	9.325	80.213	1.00	41.44	B
	ATOM	3254	N	ILE	B	553	78.160	8.579	78.093	1.00	41.46	B
	ATOM	3255	CA	ILE	B	553	79.589	8.788	77.879	1.00	41.69	B
	ATOM	3256	CB	ILE	B	553	80.366	7.452	77.679	1.00	41.75	B
20	ATOM	3257	CG2	ILE	B	553	81.854	7.746	77.598	1.00	41.32	B
	ATOM	3258	CG1	ILE	B	553	80.077	6.451	78.811	1.00	42.93	B
	ATOM	3259	CD1	ILE	B	553	80.616	6.835	80.176	1.00	42.43	B
	ATOM	3260	C	ILE	B	553	79.774	9.615	76.612	1.00	41.85	B
	ATOM	3261	O	ILE	B	553	79.057	9.419	75.631	1.00	41.17	B
25	ATOM	3262	N	VAL	B	554	80.724	10.547	76.638	1.00	42.67	B
	ATOM	3263	CA	VAL	B	554	81.022	11.371	75.467	1.00	43.83	B
	ATOM	3264	CB	VAL	B	554	81.216	12.850	75.832	1.00	43.23	B
	ATOM	3265	CG1	VAL	B	554	81.219	13.690	74.566	1.00	41.99	B
	ATOM	3266	CG2	VAL	B	554	80.143	13.294	76.799	1.00	43.78	B
30	ATOM	3267	C	VAL	B	554	82.344	10.858	74.907	1.00	44.98	B
	ATOM	3268	O	VAL	B	554	83.391	11.108	75.489	1.00	45.12	B
	ATOM	3269	N	TRP	B	555	82.305	10.152	73.782	1.00	46.53	B
	ATOM	3270	CA	TRP	B	555	83.526	9.603	73.198	1.00	48.33	B
	ATOM	3271	CB	TRP	B	555	83.264	8.193	72.652	1.00	48.73	B
35	ATOM	3272	CG	TRP	B	555	82.491	7.287	73.562	1.00	48.42	B
	ATOM	3273	CD2	TRP	B	555	83.024	6.244	74.390	1.00	49.05	B
	ATOM	3274	CE2	TRP	B	555	81.934	5.644	75.060	1.00	49.51	B
	ATOM	3275	CE3	TRP	B	555	84.317	5.758	74.629	1.00	48.35	B
	ATOM	3276	CD1	TRP	B	555	81.140	7.281	73.762	1.00	48.53	B
40	ATOM	3277	NE1	TRP	B	555	80.797	6.296	74.661	1.00	49.31	B
	ATOM	3278	CZ2	TRP	B	555	82.099	4.579	75.958	1.00	49.91	B
	ATOM	3279	CZ3	TRP	B	555	84.481	4.698	75.523	1.00	47.73	B
	ATOM	3280	CH2	TRP	B	555	83.378	4.121	76.174	1.00	48.67	B
	ATOM	3281	C	TRP	B	555	84.119	10.455	72.074	1.00	49.09	B
45	ATOM	3282	O	TRP	B	555	83.424	11.253	71.451	1.00	48.46	B
	ATOM	3283	N	ASP	B	556	85.411	10.265	71.816	1.00	51.15	B
	ATOM	3284	CA	ASP	B	556	86.119	10.978	70.745	1.00	52.97	B
	ATOM	3285	CB	ASP	B	556	87.358	11.705	71.295	1.00	53.47	B
	ATOM	3286	CG	ASP	B	556	88.047	12.594	70.247	1.00	53.63	B
50	ATOM	3287	OD1	ASP	B	556	88.097	12.203	69.060	1.00	52.44	B
	ATOM	3288	OD2	ASP	B	556	88.552	13.683	70.615	1.00	53.83	B
	ATOM	3289	C	ASP	B	556	86.569	9.933	69.726	1.00	53.38	B
	ATOM	3290	O	ASP	B	556	87.740	9.560	69.688	1.00	54.18	B
	ATOM	3291	N	VAL	B	557	85.635	9.460	68.909	1.00	54.03	B

```
ATOM   3292  CA  VAL B 557      85.925   8.446  67.896  1.00 53.93      B
ATOM   3293  CB  VAL B 557      84.859   8.493  66.780  1.00 53.70      B
ATOM   3294  CG1 VAL B 557      85.210   7.519  65.660  1.00 54.83      B
ATOM   3295  CG2 VAL B 557      83.502   8.151  67.370  1.00 52.75      B
ATOM   3296  C   VAL B 557      87.327   8.578  67.295  1.00 54.01      B
ATOM   3297  O   VAL B 557      88.014   7.575  67.065  1.00 53.12      B
ATOM   3298  N   ALA B 558      87.752   9.817  67.063  1.00 54.57      B
ATOM   3299  CA  ALA B 558      89.071  10.087  66.497  1.00 55.27      B
ATOM   3300  CB  ALA B 558      89.249  11.577  66.286  1.00 54.44      B
ATOM   3301  C   ALA B 558      90.189   9.554  67.393  1.00 56.09      B
ATOM   3302  O   ALA B 558      91.154   8.948  66.917  1.00 57.14      B
ATOM   3303  N   GLN B 559      90.054   9.779  68.693  1.00 56.27      B
ATOM   3304  CA  GLN B 559      91.052   9.325  69.652  1.00 56.00      B
ATOM   3305  CB  GLN B 559      91.358  10.445  70.643  1.00 57.58      B
ATOM   3306  CG  GLN B 559      91.679  11.771  69.977  1.00 60.76      B
ATOM   3307  CD  GLN B 559      92.288  12.773  70.944  1.00 63.21      B
ATOM   3308  OE1 GLN B 559      91.798  12.942  72.072  1.00 63.29      B
ATOM   3309  NE2 GLN B 559      93.360  13.449  70.510  1.00 62.95      B
ATOM   3310  C   GLN B 559      90.556   8.090  70.400  1.00 54.82      B
ATOM   3311  O   GLN B 559      91.131   7.679  71.407  1.00 53.08      B
ATOM   3312  N   MSE B 560      89.486   7.500  69.885  1.00 54.44      B
ATOM   3313  CA  MSE B 560      88.881   6.322  70.487  1.00 54.74      B
ATOM   3314  CB  MSE B 560      89.450   5.055  69.844  1.00 54.65      B
ATOM   3315  CG  MSE B 560      89.124   4.912  68.360  1.00 54.73      B
ATOM   3316  SE  MSE B 560      87.225   4.845  67.991  1.00 57.83      B
ATOM   3317  CE  MSE B 560      86.882   2.985  68.379  1.00 53.96      B
ATOM   3318  C   MSE B 560      89.041   6.275  72.013  1.00 54.33      B
ATOM   3319  O   MSE B 560      89.330   5.230  72.600  1.00 54.09      B
ATOM   3320  N   LYS B 561      88.838   7.419  72.654  1.00 53.76      B
ATOM   3321  CA  LYS B 561      88.945   7.494  74.100  1.00 53.03      B
ATOM   3322  CB  LYS B 561      90.168   8.331  74.473  0.00 53.61      B
ATOM   3323  CG  LYS B 561      90.538   8.294  75.933  0.00 54.07      B
ATOM   3324  CD  LYS B 561      91.867   8.981  76.146  0.00 54.52      B
ATOM   3325  CE  LYS B 561      92.219   9.039  77.612  0.00 54.82      B
ATOM   3326  NZ  LYS B 561      91.225   9.852  78.361  0.00 55.11      B
ATOM   3327  C   LYS B 561      87.663   8.092  74.690  1.00 52.48      B
ATOM   3328  O   LYS B 561      86.786   8.548  73.952  1.00 53.43      B
ATOM   3329  N   CYS B 562      87.553   8.063  76.018  1.00 50.98      B
ATOM   3330  CA  CYS B 562      86.394   8.601  76.740  1.00 48.94      B
ATOM   3331  CB  CYS B 562      86.209   7.834  78.056  1.00 49.61      B
ATOM   3332  SG  CYS B 562      85.037   8.536  79.259  1.00 51.47      B
ATOM   3333  C   CYS B 562      86.646  10.076  77.029  1.00 47.64      B
ATOM   3334  O   CYS B 562      87.772  10.450  77.339  1.00 48.22      B
ATOM   3335  N   LEU B 563      85.616  10.915  76.909  1.00 46.12      B
ATOM   3336  CA  LEU B 563      85.771  12.346  77.175  1.00 44.98      B
ATOM   3337  CB  LEU B 563      85.149  13.187  76.051  1.00 44.96      B
ATOM   3338  CG  LEU B 563      85.894  13.179  74.706  1.00 46.73      B
ATOM   3339  CD1 LEU B 563      85.234  14.142  73.721  1.00 45.90      B
ATOM   3340  CD2 LEU B 563      87.346  13.583  74.931  1.00 45.81      B
ATOM   3341  C   LEU B 563      85.165  12.731  78.518  1.00 43.88      B
ATOM   3342  O   LEU B 563      85.823  13.367  79.348  1.00 43.62      B
ATOM   3343  N   TYR B 564      83.913  12.345  78.731  1.00 42.63      B
ATOM   3344  CA  TYR B 564      83.244  12.632  79.986  1.00 41.64      B
ATOM   3345  CB  TYR B 564      82.429  13.918  79.887  1.00 41.63      B
```

```
ATOM   3346  CG  TYR B 564      83.248  15.149  79.592  1.00 42.86      B
ATOM   3347  CD1 TYR B 564      83.298  15.684  78.308  1.00 43.33      B
ATOM   3348  CE1 TYR B 564      84.049  16.819  78.036  1.00 45.08      B
ATOM   3349  CD2 TYR B 564      83.976  15.782  80.602  1.00 43.76      B
ATOM   3350  CE2 TYR B 564      84.732  16.916  80.341  1.00 43.78      B
ATOM   3351  CZ  TYR B 564      84.760  17.426  79.060  1.00 46.05      B
ATOM   3352  OH  TYR B 564      85.492  18.558  78.795  1.00 48.58      B
ATOM   3353  C   TYR B 564      82.321  11.491  80.356  1.00 41.77      B
ATOM   3354  O   TYR B 564      81.899  10.722  79.489  1.00 42.27      B
ATOM   3355  N   ILE B 565      82.011  11.391  81.647  1.00 41.33      B
ATOM   3356  CA  ILE B 565      81.116  10.358  82.156  1.00 40.82      B
ATOM   3357  CB  ILE B 565      81.828   9.414  83.169  1.00 41.48      B
ATOM   3358  CG2 ILE B 565      80.934   8.234  83.486  1.00 40.38      B
ATOM   3359  CG1 ILE B 565      83.126   8.862  82.582  1.00 40.59      B
ATOM   3360  CD1 ILE B 565      83.907   8.008  83.571  1.00 41.08      B
ATOM   3361  C   ILE B 565      79.938  11.020  82.860  1.00 40.09      B
ATOM   3362  O   ILE B 565      79.853  11.020  84.089  1.00 41.84      B
ATOM   3363  N   LEU B 566      79.033  11.582  82.067  1.00 38.80      B
ATOM   3364  CA  LEU B 566      77.841  12.256  82.580  1.00 36.98      B
ATOM   3365  CB  LEU B 566      76.990  12.754  81.421  1.00 36.01      B
ATOM   3366  CG  LEU B 566      77.792  13.369  80.272  1.00 35.51      B
ATOM   3367  CD1 LEU B 566      76.846  13.709  79.138  1.00 34.67      B
ATOM   3368  CD2 LEU B 566      78.541  14.592  80.757  1.00 33.68      B
ATOM   3369  C   LEU B 566      77.010  11.306  83.411  1.00 36.96      B
ATOM   3370  O   LEU B 566      76.354  10.414  82.877  1.00 36.93      B
ATOM   3371  N   SER B 567      77.021  11.498  84.721  1.00 37.95      B
ATOM   3372  CA  SER B 567      76.252  10.628  85.601  1.00 39.30      B
ATOM   3373  CB  SER B 567      77.191   9.655  86.305  1.00 39.73      B
ATOM   3374  OG  SER B 567      78.238  10.359  86.940  1.00 40.54      B
ATOM   3375  C   SER B 567      75.466  11.417  86.635  1.00 39.56      B
ATOM   3376  O   SER B 567      76.007  12.260  87.344  1.00 39.82      B
ATOM   3377  N   GLY B 568      74.181  11.116  86.728  1.00 40.79      B
ATOM   3378  CA  GLY B 568      73.338  11.798  87.685  1.00 40.25      B
ATOM   3379  C   GLY B 568      71.949  11.190  87.704  1.00 40.41      B
ATOM   3380  O   GLY B 568      71.270  11.232  88.723  1.00 41.14      B
ATOM   3381  N   HIS B 569      71.513  10.636  86.575  1.00 40.65      B
ATOM   3382  CA  HIS B 569      70.197  10.017  86.508  1.00 40.96      B
ATOM   3383  CB  HIS B 569      69.865   9.568  85.077  1.00 40.33      B
ATOM   3384  CG  HIS B 569      69.511  10.695  84.151  1.00 40.43      B
ATOM   3385  CD2 HIS B 569      68.558  11.657  84.232  1.00 39.98      B
ATOM   3386  ND1 HIS B 569      70.194  10.936  82.977  1.00 40.06      B
ATOM   3387  CE1 HIS B 569      69.681  11.995  82.378  1.00 38.53      B
ATOM   3388  NE2 HIS B 569      68.687  12.452  83.118  1.00 38.90      B
ATOM   3389  C   HIS B 569      70.193   8.822  87.448  1.00 40.82      B
ATOM   3390  O   HIS B 569      71.239   8.242  87.743  1.00 39.68      B
ATOM   3391  N   THR B 570      69.007   8.464  87.915  1.00 41.28      B
ATOM   3392  CA  THR B 570      68.857   7.364  88.838  1.00 41.75      B
ATOM   3393  CB  THR B 570      68.025   7.806  90.042  1.00 42.58      B
ATOM   3394  OG1 THR B 570      68.417   9.135  90.414  1.00 41.17      B
ATOM   3395  CG2 THR B 570      68.265   6.872  91.226  1.00 44.09      B
ATOM   3396  C   THR B 570      68.201   6.169  88.168  1.00 41.63      B
ATOM   3397  O   THR B 570      67.554   5.348  88.824  1.00 42.87      B
ATOM   3398  N   ASP B 571      68.348   6.087  86.852  1.00 40.41      B
ATOM   3399  CA  ASP B 571      67.795   4.969  86.116  1.00 38.73      B
```

```
ATOM   3400  CB  ASP B 571      66.273   4.960  86.200  1.00 37.92      B
ATOM   3401  CG  ASP B 571      65.726   3.569  86.446  1.00 38.68      B
ATOM   3402  OD1 ASP B 571      66.270   2.616  85.852  1.00 37.31      B
ATOM   3403  OD2 ASP B 571      64.757   3.425  87.225  1.00 39.84      B
ATOM   3404  C   ASP B 571      68.240   4.941  84.663  1.00 38.21      B
ATOM   3405  O   ASP B 571      68.800   5.914  84.147  1.00 37.05      B
ATOM   3406  N   ARG B 572      67.994   3.806  84.016  1.00 38.06      B
ATOM   3407  CA  ARG B 572      68.365   3.602  82.620  1.00 38.61      B
ATOM   3408  CB  ARG B 572      67.761   2.282  82.102  1.00 39.79      B
ATOM   3409  CG  ARG B 572      66.409   1.944  82.735  1.00 42.08      B
ATOM   3410  CD  ARG B 572      65.669   0.771  82.066  1.00 43.20      B
ATOM   3411  NE  ARG B 572      66.402  -0.497  82.046  1.00 42.53      B
ATOM   3412  CZ  ARG B 572      65.859  -1.671  81.722  1.00 42.93      B
ATOM   3413  NH1 ARG B 572      64.573  -1.757  81.395  1.00 41.39      B
ATOM   3414  NH2 ARG B 572      66.605  -2.764  81.708  1.00 43.19      B
ATOM   3415  C   ARG B 572      67.961   4.764  81.712  1.00 37.29      B
ATOM   3416  O   ARG B 572      66.923   5.408  81.911  1.00 37.19      B
ATOM   3417  N   ILE B 573      68.803   5.022  80.716  1.00 34.87      B
ATOM   3418  CA  ILE B 573      68.589   6.088  79.739  1.00 32.30      B
ATOM   3419  CB  ILE B 573      69.914   6.783  79.417  1.00 31.72      B
ATOM   3420  CG2 ILE B 573      69.736   7.751  78.276  1.00 29.59      B
ATOM   3421  CG1 ILE B 573      70.434   7.465  80.678  1.00 33.36      B
ATOM   3422  CD1 ILE B 573      71.875   7.918  80.574  1.00 34.32      B
ATOM   3423  C   ILE B 573      68.024   5.489  78.454  1.00 30.51      B
ATOM   3424  O   ILE B 573      68.467   4.441  78.009  1.00 29.57      B
ATOM   3425  N   TYR B 574      67.039   6.148  77.862  1.00 29.36      B
ATOM   3426  CA  TYR B 574      66.453   5.629  76.638  1.00 29.00      B
ATOM   3427  CB  TYR B 574      64.944   5.478  76.795  1.00 29.33      B
ATOM   3428  CG  TYR B 574      64.557   4.229  77.537  1.00 31.08      B
ATOM   3429  CD1 TYR B 574      65.140   3.926  78.754  1.00 33.15      B
ATOM   3430  CE1 TYR B 574      64.782   2.797  79.465  1.00 33.55      B
ATOM   3431  CD2 TYR B 574      63.596   3.358  77.036  1.00 32.28      B
ATOM   3432  CE2 TYR B 574      63.225   2.209  77.748  1.00 32.21      B
ATOM   3433  CZ  TYR B 574      63.828   1.947  78.970  1.00 32.73      B
ATOM   3434  OH  TYR B 574      63.457   0.871  79.743  1.00 34.36      B
ATOM   3435  C   TYR B 574      66.745   6.452  75.393  1.00 28.82      B
ATOM   3436  O   TYR B 574      66.611   5.965  74.264  1.00 28.32      B
ATOM   3437  N   SER B 575      67.169   7.692  75.590  1.00 28.07      B
ATOM   3438  CA  SER B 575      67.431   8.564  74.461  1.00 27.39      B
ATOM   3439  CB  SER B 575      66.101   9.147  73.980  1.00 27.09      B
ATOM   3440  OG  SER B 575      66.260   9.948  72.833  1.00 23.40      B
ATOM   3441  C   SER B 575      68.368   9.690  74.832  1.00 27.21      B
ATOM   3442  O   SER B 575      68.400  10.124  75.979  1.00 29.42      B
ATOM   3443  N   THR B 576      69.131  10.169  73.859  1.00 26.42      B
ATOM   3444  CA  THR B 576      70.036  11.279  74.101  1.00 24.44      B
ATOM   3445  CB  THR B 576      71.350  10.794  74.680  1.00 23.42      B
ATOM   3446  OG1 THR B 576      72.176  11.925  74.958  1.00 22.28      B
ATOM   3447  CG2 THR B 576      72.070   9.898  73.680  1.00 23.95      B
ATOM   3448  C   THR B 576      70.314  11.995  72.782  1.00 24.66      B
ATOM   3449  O   THR B 576      70.225  11.405  71.712  1.00 23.66      B
ATOM   3450  N   ILE B 577      70.639  13.274  72.843  1.00 25.19      B
ATOM   3451  CA  ILE B 577      70.938  13.979  71.615  1.00 24.85      B
ATOM   3452  CB  ILE B 577      69.767  14.869  71.172  1.00 23.89      B
ATOM   3453  CG2 ILE B 577      70.271  15.939  70.202  1.00 21.80      B
```

```
ATOM   3454  CG1 ILE B 577      68.671  14.011  70.538  1.00 23.81      B
ATOM   3455  CD1 ILE B 577      67.376  14.750  70.224  1.00 21.31      B
ATOM   3456  C   ILE B 577      72.163  14.851  71.802  1.00 26.44      B
ATOM   3457  O   ILE B 577      72.324  15.497  72.833  1.00 26.92      B
ATOM   3458  N   TYR B 578      73.037  14.850  70.802  1.00 27.45      B
ATOM   3459  CA  TYR B 578      74.235  15.672  70.848  1.00 27.93      B
ATOM   3460  CB  TYR B 578      75.423  14.925  70.226  1.00 28.17      B
ATOM   3461  CG  TYR B 578      76.688  15.757  70.084  1.00 30.25      B
ATOM   3462  CD1 TYR B 578      77.096  16.629  71.089  1.00 28.62      B
ATOM   3463  CE1 TYR B 578      78.235  17.416  70.934  1.00 29.38      B
ATOM   3464  CD2 TYR B 578      77.464  15.690  68.922  1.00 31.91      B
ATOM   3465  CE2 TYR B 578      78.607  16.476  68.762  1.00 30.14      B
ATOM   3466  CZ  TYR B 578      78.980  17.334  69.767  1.00 29.57      B
ATOM   3467  OH  TYR B 578      80.082  18.135  69.605  1.00 31.32      B
ATOM   3468  C   TYR B 578      73.943  16.980  70.117  1.00 27.87      B
ATOM   3469  O   TYR B 578      73.789  17.017  68.897  1.00 27.54      B
ATOM   3470  N   ASP B 579      73.832  18.045  70.901  1.00 28.90      B
ATOM   3471  CA  ASP B 579      73.551  19.369  70.380  1.00 30.92      B
ATOM   3472  CB  ASP B 579      72.799  20.203  71.416  1.00 30.53      B
ATOM   3473  CG  ASP B 579      72.248  21.473  70.839  1.00 34.02      B
ATOM   3474  OD1 ASP B 579      72.845  21.995  69.868  1.00 35.60      B
ATOM   3475  OD2 ASP B 579      71.219  21.968  71.357  1.00 37.17      B
ATOM   3476  C   ASP B 579      74.871  20.026  70.035  1.00 31.94      B
ATOM   3477  O   ASP B 579      75.344  20.923  70.732  1.00 30.49      B
ATOM   3478  N   HIS B 580      75.461  19.557  68.945  1.00 34.88      B
ATOM   3479  CA  HIS B 580      76.731  20.085  68.492  1.00 38.67      B
ATOM   3480  CB  HIS B 580      77.133  19.422  67.170  1.00 40.80      B
ATOM   3481  CG  HIS B 580      76.123  19.579  66.080  1.00 44.94      B
ATOM   3482  CD2 HIS B 580      76.268  19.900  64.773  1.00 46.55      B
ATOM   3483  ND1 HIS B 580      74.778  19.359  66.276  1.00 47.64      B
ATOM   3484  CE1 HIS B 580      74.135  19.532  65.132  1.00 47.95      B
ATOM   3485  NE2 HIS B 580      75.016  19.860  64.206  1.00 46.75      B
ATOM   3486  C   HIS B 580      76.684  21.601  68.364  1.00 39.17      B
ATOM   3487  O   HIS B 580      77.545  22.297  68.907  1.00 40.61      B
ATOM   3488  N   GLU B 581      75.673  22.122  67.681  1.00 39.97      B
ATOM   3489  CA  GLU B 581      75.563  23.566  67.529  1.00 40.63      B
ATOM   3490  CB  GLU B 581      74.162  23.960  67.078  1.00 42.60      B
ATOM   3491  CG  GLU B 581      73.991  25.469  66.960  1.00 46.26      B
ATOM   3492  CD  GLU B 581      72.848  25.853  66.052  1.00 47.68      B
ATOM   3493  OE1 GLU B 581      72.857  25.407  64.880  1.00 48.93      B
ATOM   3494  OE2 GLU B 581      71.952  26.598  66.508  1.00 48.37      B
ATOM   3495  C   GLU B 581      75.871  24.279  68.836  1.00 40.05      B
ATOM   3496  O   GLU B 581      76.810  25.063  68.916  1.00 40.37      B
ATOM   3497  N   ARG B 582      75.074  23.998  69.859  1.00 39.74      B
ATOM   3498  CA  ARG B 582      75.266  24.622  71.151  1.00 38.74      B
ATOM   3499  CB  ARG B 582      73.939  24.647  71.899  1.00 37.10      B
ATOM   3500  CG  ARG B 582      73.131  25.905  71.619  1.00 37.06      B
ATOM   3501  CD  ARG B 582      71.654  25.749  71.970  1.00 35.83      B
ATOM   3502  NE  ARG B 582      70.962  24.890  71.012  1.00 35.08      B
ATOM   3503  CZ  ARG B 582      70.041  25.312  70.154  1.00 34.96      B
ATOM   3504  NH1 ARG B 582      69.691  26.591  70.130  1.00 32.75      B
ATOM   3505  NH2 ARG B 582      69.466  24.448  69.327  1.00 35.91      B
ATOM   3506  C   ARG B 582      76.356  23.971  71.989  1.00 39.71      B
ATOM   3507  O   ARG B 582      76.775  24.529  73.003  1.00 40.75      B
```

```
ATOM   3508  N   LYS B 583      76.825  22.804  71.548  1.00 40.22      B
ATOM   3509  CA  LYS B 583      77.881  22.056  72.240  1.00 39.65      B
ATOM   3510  CB  LYS B 583      79.089  22.961  72.487  1.00 41.30      B
ATOM   3511  CG  LYS B 583      80.401  22.212  72.649  1.00 43.06      B
ATOM   3512  CD  LYS B 583      80.866  21.664  71.311  1.00 46.02      B
ATOM   3513  CE  LYS B 583      81.196  22.806  70.367  1.00 46.16      B
ATOM   3514  NZ  LYS B 583      82.256  23.657  70.976  1.00 46.38      B
ATOM   3515  C   LYS B 583      77.357  21.524  73.574  1.00 38.48      B
ATOM   3516  O   LYS B 583      77.990  21.689  74.615  1.00 37.90      B
ATOM   3517  N   ARG B 584      76.202  20.871  73.526  1.00 36.80      B
ATOM   3518  CA  ARG B 584      75.575  20.343  74.728  1.00 36.72      B
ATOM   3519  CB  ARG B 584      74.436  21.278  75.140  1.00 35.58      B
ATOM   3520  CG  ARG B 584      74.930  22.481  75.916  1.00 38.40      B
ATOM   3521  CD  ARG B 584      74.542  23.820  75.330  1.00 37.40      B
ATOM   3522  NE  ARG B 584      73.160  24.166  75.635  1.00 39.31      B
ATOM   3523  CZ  ARG B 584      72.723  25.408  75.833  1.00 40.87      B
ATOM   3524  NH1 ARG B 584      73.556  26.437  75.759  1.00 40.61      B
ATOM   3525  NH2 ARG B 584      71.448  25.617  76.122  1.00 40.77      B
ATOM   3526  C   ARG B 584      75.045  18.915  74.573  1.00 36.65      B
ATOM   3527  O   ARG B 584      75.211  18.298  73.522  1.00 36.06      B
ATOM   3528  N   CYS B 585      74.443  18.372  75.631  1.00 36.04      B
ATOM   3529  CA  CYS B 585      73.847  17.043  75.534  1.00 34.78      B
ATOM   3530  CB  CYS B 585      74.778  15.936  75.994  1.00 36.01      B
ATOM   3531  SG  CYS B 585      73.955  14.322  75.938  1.00 38.57      B
ATOM   3532  C   CYS B 585      72.566  16.929  76.330  1.00 33.64      B
ATOM   3533  O   CYS B 585      72.503  17.328  77.495  1.00 33.83      B
ATOM   3534  N   ILE B 586      71.544  16.397  75.668  1.00 31.40      B
ATOM   3535  CA  ILE B 586      70.247  16.182  76.277  1.00 31.62      B
ATOM   3536  CB  ILE B 586      69.079  16.610  75.325  1.00 29.83      B
ATOM   3537  CG2 ILE B 586      67.725  16.305  75.961  1.00 25.17      B
ATOM   3538  CG1 ILE B 586      69.155  18.111  75.009  1.00 28.59      B
ATOM   3539  CD1 ILE B 586      69.610  18.438  73.588  1.00 27.79      B
ATOM   3540  C   ILE B 586      70.135  14.680  76.534  1.00 33.85      B
ATOM   3541  O   ILE B 586      70.530  13.882  75.679  1.00 35.25      B
ATOM   3542  N   SER B 587      69.634  14.291  77.712  1.00 34.29      B
ATOM   3543  CA  SER B 587      69.428  12.870  78.031  1.00 34.28      B
ATOM   3544  CB  SER B 587      70.548  12.320  78.933  1.00 33.74      B
ATOM   3545  OG  SER B 587      70.727  13.066  80.122  1.00 34.80      B
ATOM   3546  C   SER B 587      68.060  12.648  78.685  1.00 33.99      B
ATOM   3547  O   SER B 587      67.639  13.419  79.546  1.00 32.52      B
ATOM   3548  N   ALA B 588      67.355  11.615  78.233  1.00 34.19      B
ATOM   3549  CA  ALA B 588      66.054  11.286  78.793  1.00 35.71      B
ATOM   3550  CB  ALA B 588      65.006  11.155  77.699  1.00 35.73      B
ATOM   3551  C   ALA B 588      66.259   9.960  79.495  1.00 36.25      B
ATOM   3552  O   ALA B 588      66.752   9.016  78.884  1.00 37.28      B
ATOM   3553  N   SER B 589      65.929   9.906  80.786  1.00 36.81      B
ATOM   3554  CA  SER B 589      66.084   8.684  81.582  1.00 35.90      B
ATOM   3555  CB  SER B 589      66.888   8.950  82.851  1.00 34.91      B
ATOM   3556  OG  SER B 589      66.512   8.030  83.870  1.00 32.54      B
ATOM   3557  C   SER B 589      64.761   8.093  82.005  1.00 35.49      B
ATOM   3558  O   SER B 589      63.714   8.712  81.844  1.00 34.24      B
ATOM   3559  N   MSE B 590      64.826   6.883  82.550  1.00 36.42      B
ATOM   3560  CA  MSE B 590      63.648   6.188  83.040  1.00 36.64      B
ATOM   3561  CB  MSE B 590      63.949   4.702  83.249  1.00 39.18      B
```

```
ATOM   3562  CG  MSE B 590      62.896   3.948  84.060  1.00 41.10      B
ATOM   3563  SE  MSE B 590      63.091   2.012  83.900  1.00 46.30      B
ATOM   3564  CE  MSE B 590      61.725   1.645  82.565  1.00 45.20      B
ATOM   3565  C   MSE B 590      63.241   6.819  84.361  1.00 35.83      B
ATOM   3566  O   MSE B 590      62.152   6.554  84.860  1.00 35.48      B
ATOM   3567  N   ASP B 591      64.116   7.650  84.932  1.00 35.51      B
ATOM   3568  CA  ASP B 591      63.791   8.301  86.198  1.00 34.59      B
ATOM   3569  CB  ASP B 591      65.051   8.767  86.951  1.00 34.80      B
ATOM   3570  CG  ASP B 591      65.874   9.763  86.177  1.00 34.10      B
ATOM   3571  OD1 ASP B 591      65.329  10.459  85.300  1.00 35.66      B
ATOM   3572  OD2 ASP B 591      67.081   9.869  86.466  1.00 33.64      B
ATOM   3573  C   ASP B 591      62.838   9.463  85.986  1.00 33.76      B
ATOM   3574  O   ASP B 591      62.767  10.373  86.801  1.00 31.76      B
ATOM   3575  N   THR B 592      62.120   9.418  84.866  1.00 35.29      B
ATOM   3576  CA  THR B 592      61.120  10.419  84.536  1.00 34.85      B
ATOM   3577  CB  THR B 592      59.984  10.372  85.631  1.00 34.66      B
ATOM   3578  OG1 THR B 592      58.742  10.820  85.079  1.00 38.41      B
ATOM   3579  CG2 THR B 592      60.338  11.235  86.830  1.00 34.65      B
ATOM   3580  C   THR B 592      61.745  11.811  84.403  1.00 33.52      B
ATOM   3581  O   THR B 592      61.049  12.815  84.455  1.00 33.23      B
ATOM   3582  N   THR B 593      63.053  11.858  84.169  1.00 32.55      B
ATOM   3583  CA  THR B 593      63.764  13.130  84.070  1.00 32.86      B
ATOM   3584  CB  THR B 593      64.786  13.239  85.217  1.00 34.19      B
ATOM   3585  OG1 THR B 593      64.082  13.389  86.454  1.00 36.50      B
ATOM   3586  CG2 THR B 593      65.730  14.430  85.018  1.00 38.69      B
ATOM   3587  C   THR B 593      64.500  13.423  82.765  1.00 33.21      B
ATOM   3588  O   THR B 593      64.856  12.519  82.015  1.00 32.79      B
ATOM   3589  N   ILE B 594      64.714  14.705  82.488  1.00 33.30      B
ATOM   3590  CA  ILE B 594      65.471  15.103  81.309  1.00 33.34      B
ATOM   3591  CB  ILE B 594      64.612  15.829  80.249  1.00 31.46      B
ATOM   3592  CG2 ILE B 594      65.496  16.322  79.132  1.00 29.37      B
ATOM   3593  CG1 ILE B 594      63.534  14.902  79.690  1.00 32.39      B
ATOM   3594  CD1 ILE B 594      62.436  15.642  78.920  1.00 27.89      B
ATOM   3595  C   ILE B 594      66.497  16.104  81.824  1.00 35.21      B
ATOM   3596  O   ILE B 594      66.161  16.973  82.628  1.00 37.01      B
ATOM   3597  N   ARG B 595      67.749  15.977  81.402  1.00 35.67      B
ATOM   3598  CA  ARG B 595      68.735  16.947  81.834  1.00 36.60      B
ATOM   3599  CB  ARG B 595      69.447  16.482  83.104  1.00 39.57      B
ATOM   3600  CG  ARG B 595      70.237  15.219  83.020  1.00 41.84      B
ATOM   3601  CD  ARG B 595      70.672  14.865  84.428  1.00 43.91      B
ATOM   3602  NE  ARG B 595      69.554  14.397  85.240  1.00 44.22      B
ATOM   3603  CZ  ARG B 595      69.658  14.054  86.518  1.00 45.26      B
ATOM   3604  NH1 ARG B 595      70.848  14.147  87.121  1.00 44.50      B
ATOM   3605  NH2 ARG B 595      68.586  13.589  87.170  1.00 41.38      B
ATOM   3606  C   ARG B 595      69.731  17.324  80.751  1.00 36.11      B
ATOM   3607  O   ARG B 595      70.067  16.512  79.880  1.00 36.08      B
ATOM   3608  N   ILE B 596      70.173  18.579  80.791  1.00 34.47      B
ATOM   3609  CA  ILE B 596      71.116  19.084  79.807  1.00 34.38      B
ATOM   3610  CB  ILE B 596      70.662  20.479  79.263  1.00 35.15      B
ATOM   3611  CG2 ILE B 596      71.746  21.058  78.357  1.00 35.63      B
ATOM   3612  CG1 ILE B 596      69.390  20.334  78.401  1.00 36.12      B
ATOM   3613  CD1 ILE B 596      68.175  19.723  79.073  1.00 29.57      B
ATOM   3614  C   ILE B 596      72.515  19.174  80.415  1.00 32.98      B
ATOM   3615  O   ILE B 596      72.679  19.563  81.570  1.00 30.78      B
```

```
ATOM   3616  N   TRP B 597      73.520  18.795  79.638  1.00 33.10      B
ATOM   3617  CA  TRP B 597      74.892  18.821  80.124  1.00 34.71      B
ATOM   3618  CB  TRP B 597      75.493  17.404  80.117  1.00 34.39      B
ATOM   3619  CG  TRP B 597      74.577  16.341  80.645  1.00 33.10      B
ATOM   3620  CD2 TRP B 597      74.691  15.653  81.893  1.00 33.20      B
ATOM   3621  CE2 TRP B 597      73.607  14.752  81.974  1.00 33.38      B
ATOM   3622  CE3 TRP B 597      75.599  15.713  82.956  1.00 33.08      B
ATOM   3623  CD1 TRP B 597      73.463  15.842  80.035  1.00 33.47      B
ATOM   3624  NE1 TRP B 597      72.874  14.884  80.826  1.00 32.94      B
ATOM   3625  CZ2 TRP B 597      73.411  13.912  83.072  1.00 33.63      B
ATOM   3626  CZ3 TRP B 597      75.406  14.878  84.051  1.00 32.87      B
ATOM   3627  CH2 TRP B 597      74.314  13.989  84.101  1.00 33.13      B
ATOM   3628  C   TRP B 597      75.725  19.726  79.229  1.00 35.90      B
ATOM   3629  O   TRP B 597      75.455  19.837  78.028  1.00 36.19      B
ATOM   3630  N   ASP B 598      76.731  20.372  79.817  1.00 36.61      B
ATOM   3631  CA  ASP B 598      77.631  21.265  79.082  1.00 38.19      B
ATOM   3632  CB  ASP B 598      78.156  22.369  80.018  1.00 36.98      B
ATOM   3633  CG  ASP B 598      78.999  23.410  79.291  1.00 37.20      B
ATOM   3634  OD1 ASP B 598      79.604  23.089  78.240  1.00 36.53      B
ATOM   3635  OD2 ASP B 598      79.059  24.553  79.786  1.00 37.52      B
ATOM   3636  C   ASP B 598      78.806  20.426  78.574  1.00 39.00      B
ATOM   3637  O   ASP B 598      79.670  20.050  79.349  1.00 39.73      B
ATOM   3638  N   LEU B 599      78.847  20.126  77.282  1.00 40.71      B
ATOM   3639  CA  LEU B 599      79.942  19.320  76.747  1.00 42.08      B
ATOM   3640  CB  LEU B 599      79.593  18.805  75.344  1.00 40.52      B
ATOM   3641  CG  LEU B 599      78.606  17.628  75.251  1.00 40.62      B
ATOM   3642  CD1 LEU B 599      79.264  16.437  74.600  1.00 38.01      B
ATOM   3643  CD2 LEU B 599      78.096  17.258  76.638  1.00 38.10      B
ATOM   3644  C   LEU B 599      81.295  20.025  76.721  1.00 43.84      B
ATOM   3645  O   LEU B 599      82.256  19.494  76.165  1.00 44.70      B
ATOM   3646  N   GLU B 600      81.373  21.216  77.315  1.00 44.72      B
ATOM   3647  CA  GLU B 600      82.637  21.941  77.358  1.00 45.68      B
ATOM   3648  CB  GLU B 600      82.412  23.413  77.697  1.00 48.89      B
ATOM   3649  CG  GLU B 600      83.460  24.367  77.128  1.00 52.63      B
ATOM   3650  CD  GLU B 600      84.762  24.375  77.924  1.00 56.18      B
ATOM   3651  OE1 GLU B 600      84.739  24.763  79.120  1.00 58.19      B
ATOM   3652  OE2 GLU B 600      85.811  23.997  77.353  1.00 57.88      B
ATOM   3653  C   GLU B 600      83.480  21.254  78.419  1.00 45.43      B
ATOM   3654  O   GLU B 600      84.683  21.083  78.242  1.00 46.22      B
ATOM   3655  N   ASN B 605      82.844  20.855  79.518  1.00 44.31      B
ATOM   3656  CA  ASN B 605      83.543  20.124  80.568  1.00 43.89      B
ATOM   3657  CB  ASN B 605      84.285  21.077  81.520  1.00 46.09      B
ATOM   3658  CG  ASN B 605      85.808  21.121  81.248  1.00 50.14      B
ATOM   3659  OD1 ASN B 605      86.508  20.093  81.348  1.00 50.14      B
ATOM   3660  ND2 ASN B 605      86.320  22.314  80.900  1.00 49.96      B
ATOM   3661  C   ASN B 605      82.630  19.186  81.346  1.00 41.67      B
ATOM   3662  O   ASN B 605      82.756  19.054  82.554  1.00 43.82      B
ATOM   3663  N   GLY B 606      81.718  18.525  80.638  1.00 38.96      B
ATOM   3664  CA  GLY B 606      80.804  17.584  81.268  1.00 35.37      B
ATOM   3665  C   GLY B 606      80.059  18.044  82.512  1.00 34.56      B
ATOM   3666  O   GLY B 606      79.668  17.231  83.350  1.00 32.65      B
ATOM   3667  N   GLU B 607      79.846  19.348  82.622  1.00 34.50      B
ATOM   3668  CA  GLU B 607      79.147  19.921  83.757  1.00 35.96      B
ATOM   3669  CB  GLU B 607      79.616  21.367  83.976  1.00 36.06      B
```

```
ATOM   3670  CG  GLU B 607      81.114  21.618  83.763  1.00 39.20      B
ATOM   3671  CD  GLU B 607      81.468  21.981  82.321  1.00 39.57      B
ATOM   3672  OE1 GLU B 607      80.924  21.353  81.405  1.00 41.63      B
ATOM   3673  OE2 GLU B 607      82.301  22.877  82.097  1.00 38.72      B
ATOM   3674  C   GLU B 607      77.622  19.892  83.504  1.00 37.13      B
ATOM   3675  O   GLU B 607      77.157  20.165  82.391  1.00 36.86      B
ATOM   3676  N   LEU B 608      76.850  19.539  84.530  1.00 37.44      B
ATOM   3677  CA  LEU B 608      75.395  19.513  84.412  1.00 37.50      B
ATOM   3678  CB  LEU B 608      74.753  18.822  85.622  1.00 37.08      B
ATOM   3679  CG  LEU B 608      73.218  18.925  85.723  1.00 37.03      B
ATOM   3680  CD1 LEU B 608      72.593  18.036  84.658  1.00 36.12      B
ATOM   3681  CD2 LEU B 608      72.724  18.533  87.127  1.00 34.40      B
ATOM   3682  C   LEU B 608      74.912  20.962  84.339  1.00 38.65      B
ATOM   3683  O   LEU B 608      75.442  21.833  85.030  1.00 38.26      B
ATOM   3684  N   MSE B 625      73.902  21.210  83.510  1.00 39.30      B
ATOM   3685  CA  MSE B 625      73.368  22.553  83.329  1.00 39.07      B
ATOM   3686  CB  MSE B 625      73.266  22.890  81.842  1.00 41.00      B
ATOM   3687  CG  MSE B 625      74.571  23.323  81.217  1.00 43.67      B
ATOM   3688  SE  MSE B 625      74.423  23.805  79.359  1.00 50.89      B
ATOM   3689  CE  MSE B 625      73.882  25.650  79.578  1.00 45.39      B
ATOM   3690  C   MSE B 625      72.008  22.737  83.946  1.00 38.75      B
ATOM   3691  O   MSE B 625      71.803  23.605  84.795  1.00 39.63      B
ATOM   3692  N   TYR B 626      71.068  21.919  83.495  1.00 38.88      B
ATOM   3693  CA  TYR B 626      69.700  22.003  83.975  1.00 37.07      B
ATOM   3694  CB  TYR B 626      68.861  22.841  83.016  1.00 35.69      B
ATOM   3695  CG  TYR B 626      69.457  24.160  82.618  1.00 34.35      B
ATOM   3696  CD1 TYR B 626      69.560  25.199  83.535  1.00 33.06      B
ATOM   3697  CE1 TYR B 626      70.013  26.447  83.150  1.00 32.14      B
ATOM   3698  CD2 TYR B 626      69.840  24.397  81.295  1.00 34.51      B
ATOM   3699  CE2 TYR B 626      70.296  25.646  80.896  1.00 33.07      B
ATOM   3700  CZ  TYR B 626      70.373  26.671  81.833  1.00 31.79      B
ATOM   3701  OH  TYR B 626      70.753  27.933  81.446  1.00 28.57      B
ATOM   3702  C   TYR B 626      69.067  20.635  84.040  1.00 36.34      B
ATOM   3703  O   TYR B 626      69.528  19.690  83.410  1.00 37.33      B
ATOM   3704  N   THR B 627      67.992  20.560  84.809  1.00 36.28      B
ATOM   3705  CA  THR B 627      67.203  19.357  84.958  1.00 34.33      B
ATOM   3706  CB  THR B 627      67.340  18.744  86.373  1.00 32.94      B
ATOM   3707  OG1 THR B 627      68.684  18.292  86.562  1.00 30.38      B
ATOM   3708  CG2 THR B 627      66.391  17.544  86.535  1.00 32.04      B
ATOM   3709  C   THR B 627      65.764  19.808  84.719  1.00 34.24      B
ATOM   3710  O   THR B 627      65.248  20.700  85.400  1.00 33.46      B
ATOM   3711  N   LEU B 628      65.137  19.204  83.722  1.00 34.53      B
ATOM   3712  CA  LEU B 628      63.772  19.525  83.355  1.00 34.30      B
ATOM   3713  CB  LEU B 628      63.636  19.558  81.835  1.00 35.54      B
ATOM   3714  CG  LEU B 628      64.814  20.120  81.056  1.00 36.04      B
ATOM   3715  CD1 LEU B 628      64.459  20.071  79.591  1.00 37.79      B
ATOM   3716  CD2 LEU B 628      65.137  21.538  81.500  1.00 35.35      B
ATOM   3717  C   LEU B 628      62.844  18.454  83.886  1.00 32.68      B
ATOM   3718  O   LEU B 628      63.055  17.261  83.647  1.00 33.72      B
ATOM   3719  N   GLN B 629      61.805  18.882  84.582  1.00 30.62      B
ATOM   3720  CA  GLN B 629      60.849  17.949  85.127  1.00 30.70      B
ATOM   3721  CB  GLN B 629      60.774  18.082  86.647  1.00 28.58      B
ATOM   3722  CG  GLN B 629      59.867  17.050  87.257  1.00 27.57      B
ATOM   3723  CD  GLN B 629      60.402  15.655  87.063  1.00 28.68      B
```

```
ATOM   3724  OE1 GLN B 629      59.733  14.775  86.486  1.00 28.51      B
ATOM   3725  NE2 GLN B 629      61.620  15.434  87.545  1.00 27.17      B
ATOM   3726  C   GLN B 629      59.473  18.204  84.544  1.00 31.36      B
ATOM   3727  O   GLN B 629      58.677  18.958  85.104  1.00 31.90      B
ATOM   3728  N   GLY B 630      59.183  17.567  83.424  1.00 31.87      B
ATOM   3729  CA  GLY B 630      57.889  17.767  82.804  1.00 33.15      B
ATOM   3730  C   GLY B 630      57.254  16.467  82.364  1.00 33.55      B
ATOM   3731  O   GLY B 630      56.511  16.425  81.385  1.00 35.60      B
ATOM   3732  N   HIS B 631      57.553  15.400  83.092  1.00 32.53      B
ATOM   3733  CA  HIS B 631      57.023  14.083  82.784  1.00 30.78      B
ATOM   3734  CB  HIS B 631      57.943  13.368  81.792  1.00 28.27      B
ATOM   3735  CG  HIS B 631      58.054  14.052  80.466  1.00 24.31      B
ATOM   3736  CD2 HIS B 631      59.003  14.874  79.965  1.00 21.91      B
ATOM   3737  ND1 HIS B 631      57.118  13.895  79.467  1.00 26.41      B
ATOM   3738  CE1 HIS B 631      57.487  14.587  78.405  1.00 22.90      B
ATOM   3739  NE2 HIS B 631      58.629  15.190  78.681  1.00 22.42      B
ATOM   3740  C   HIS B 631      56.957  13.302  84.091  1.00 30.77      B
ATOM   3741  O   HIS B 631      57.834  13.437  84.948  1.00 30.31      B
ATOM   3742  N   THR B 632      55.916  12.489  84.239  1.00 31.40      B
ATOM   3743  CA  THR B 632      55.716  11.690  85.447  1.00 32.08      B
ATOM   3744  CB  THR B 632      54.281  11.742  85.914  1.00 32.58      B
ATOM   3745  OG1 THR B 632      53.446  11.255  84.860  1.00 33.44      B
ATOM   3746  CG2 THR B 632      53.877  13.151  86.274  1.00 31.80      B
ATOM   3747  C   THR B 632      55.990  10.233  85.152  1.00 32.55      B
ATOM   3748  O   THR B 632      55.790   9.367  86.000  1.00 33.19      B
ATOM   3749  N   ALA B 633      56.442   9.963  83.941  1.00 32.22      B
ATOM   3750  CA  ALA B 633      56.721   8.604  83.537  1.00 32.78      B
ATOM   3751  CB  ALA B 633      55.596   8.106  82.627  1.00 33.46      B
ATOM   3752  C   ALA B 633      58.048   8.649  82.786  1.00 33.18      B
ATOM   3753  O   ALA B 633      58.570   9.730  82.526  1.00 34.34      B
ATOM   3754  N   LEU B 634      58.606   7.502  82.419  1.00 32.23      B
ATOM   3755  CA  LEU B 634      59.881   7.559  81.718  1.00 31.56      B
ATOM   3756  CB  LEU B 634      60.531   6.176  81.610  1.00 32.84      B
ATOM   3757  CG  LEU B 634      59.855   5.099  80.783  1.00 33.81      B
ATOM   3758  CD1 LEU B 634      58.372   5.151  81.095  1.00 37.82      B
ATOM   3759  CD2 LEU B 634      60.122   5.300  79.304  1.00 32.77      B
ATOM   3760  C   LEU B 634      59.787   8.214  80.353  1.00 29.60      B
ATOM   3761  O   LEU B 634      58.807   8.072  79.620  1.00 27.99      B
ATOM   3762  N   VAL B 635      60.835   8.961  80.045  1.00 27.96      B
ATOM   3763  CA  VAL B 635      60.945   9.688  78.803  1.00 25.69      B
ATOM   3764  CB  VAL B 635      61.584  11.046  79.038  1.00 27.20      B
ATOM   3765  CG1 VAL B 635      61.377  11.926  77.810  1.00 28.07      B
ATOM   3766  CG2 VAL B 635      61.000  11.679  80.302  1.00 25.75      B
ATOM   3767  C   VAL B 635      61.827   8.948  77.840  1.00 23.61      B
ATOM   3768  O   VAL B 635      63.046   9.033  77.942  1.00 23.52      B
ATOM   3769  N   GLY B 636      61.219   8.248  76.891  1.00 22.88      B
ATOM   3770  CA  GLY B 636      61.998   7.488  75.928  1.00 22.35      B
ATOM   3771  C   GLY B 636      62.224   8.089  74.550  1.00 23.37      B
ATOM   3772  O   GLY B 636      62.907   7.480  73.736  1.00 24.09      B
ATOM   3773  N   LEU B 637      61.656   9.262  74.277  1.00 23.96      B
ATOM   3774  CA  LEU B 637      61.827   9.904  72.981  1.00 23.22      B
ATOM   3775  CB  LEU B 637      60.503   9.934  72.228  1.00 22.08      B
ATOM   3776  CG  LEU B 637      59.913   8.534  72.102  1.00 21.07      B
ATOM   3777  CD1 LEU B 637      58.494   8.554  71.516  1.00 18.52      B
```

```
ATOM   3778  CD2 LEU B 637      60.863   7.724  71.261  1.00 18.91      B
ATOM   3779  C   LEU B 637      62.328  11.317  73.164  1.00 25.24      B
ATOM   3780  O   LEU B 637      62.058  11.945  74.197  1.00 25.36      B
ATOM   3781  N   LEU B 638      63.048  11.797  72.142  1.00 26.06      B
ATOM   3782  CA  LEU B 638      63.635  13.147  72.077  1.00 25.52      B
ATOM   3783  CB  LEU B 638      64.907  13.258  72.926  1.00 25.76      B
ATOM   3784  CG  LEU B 638      64.857  13.321  74.453  1.00 26.07      B
ATOM   3785  CD1 LEU B 638      66.285  13.384  74.983  1.00 27.82      B
ATOM   3786  CD2 LEU B 638      64.073  14.535  74.897  1.00 25.88      B
ATOM   3787  C   LEU B 638      64.022  13.494  70.653  1.00 25.17      B
ATOM   3788  O   LEU B 638      64.529  12.644  69.919  1.00 25.44      B
ATOM   3789  N   ARG B 639      63.771  14.744  70.268  1.00 25.50      B
ATOM   3790  CA  ARG B 639      64.126  15.260  68.942  1.00 25.66      B
ATOM   3791  CB  ARG B 639      63.033  14.936  67.901  1.00 25.21      B
ATOM   3792  CG  ARG B 639      62.720  13.427  67.878  1.00 28.60      B
ATOM   3793  CD  ARG B 639      62.173  12.811  66.583  1.00 28.49      B
ATOM   3794  NE  ARG B 639      63.252  12.293  65.730  1.00 30.47      B
ATOM   3795  CZ  ARG B 639      63.131  11.295  64.851  1.00 30.02      B
ATOM   3796  NH1 ARG B 639      61.970  10.668  64.684  1.00 27.71      B
ATOM   3797  NH2 ARG B 639      64.183  10.926  64.123  1.00 32.50      B
ATOM   3798  C   ARG B 639      64.379  16.760  69.078  1.00 25.33      B
ATOM   3799  O   ARG B 639      63.738  17.442  69.877  1.00 24.41      B
ATOM   3800  N   LEU B 640      65.355  17.258  68.332  1.00 26.36      B
ATOM   3801  CA  LEU B 640      65.707  18.661  68.408  1.00 27.00      B
ATOM   3802  CB  LEU B 640      67.214  18.808  68.563  1.00 28.00      B
ATOM   3803  CG  LEU B 640      67.688  19.504  69.834  1.00 27.72      B
ATOM   3804  CD1 LEU B 640      69.188  19.757  69.737  1.00 25.31      B
ATOM   3805  CD2 LEU B 640      66.914  20.802  70.019  1.00 25.63      B
ATOM   3806  C   LEU B 640      65.263  19.432  67.189  1.00 27.04      B
ATOM   3807  O   LEU B 640      65.759  19.210  66.097  1.00 27.98      B
ATOM   3808  N   SER B 641      64.310  20.329  67.373  1.00 29.24      B
ATOM   3809  CA  SER B 641      63.828  21.138  66.271  1.00 30.57      B
ATOM   3810  CB  SER B 641      62.359  21.509  66.504  1.00 31.54      B
ATOM   3811  OG  SER B 641      62.025  22.763  65.944  1.00 30.17      B
ATOM   3812  C   SER B 641      64.718  22.366  66.277  1.00 31.05      B
ATOM   3813  O   SER B 641      65.499  22.560  67.198  1.00 32.13      B
ATOM   3814  N   ASP B 642      64.628  23.194  65.254  1.00 32.29      B
ATOM   3815  CA  ASP B 642      65.472  24.373  65.210  1.00 32.45      B
ATOM   3816  CB  ASP B 642      65.293  25.059  63.870  1.00 36.58      B
ATOM   3817  CG  ASP B 642      66.575  25.652  63.360  1.00 40.19      B
ATOM   3818  OD1 ASP B 642      67.336  24.914  62.681  1.00 41.18      B
ATOM   3819  OD2 ASP B 642      66.816  26.848  63.661  1.00 42.03      B
ATOM   3820  C   ASP B 642      65.140  25.348  66.344  1.00 31.30      B
ATOM   3821  O   ASP B 642      65.996  26.095  66.809  1.00 28.33      B
ATOM   3822  N   LYS B 643      63.876  25.332  66.759  1.00 30.65      B
ATOM   3823  CA  LYS B 643      63.373  26.190  67.818  1.00 28.54      B
ATOM   3824  CB  LYS B 643      62.069  26.888  67.407  1.00 28.11      B
ATOM   3825  CG  LYS B 643      62.141  27.807  66.210  1.00 30.60      B
ATOM   3826  CD  LYS B 643      63.196  28.902  66.364  1.00 32.54      B
ATOM   3827  CE  LYS B 643      63.332  29.736  65.070  1.00 33.58      B
ATOM   3828  NZ  LYS B 643      63.760  28.917  63.873  1.00 33.86      B
ATOM   3829  C   LYS B 643      63.047  25.391  69.077  1.00 28.15      B
ATOM   3830  O   LYS B 643      63.019  25.951  70.163  1.00 28.92      B
ATOM   3831  N   PHE B 644      62.787  24.094  68.957  1.00 26.09      B
```

```
ATOM   3832  CA  PHE B 644      62.413  23.353  70.152  1.00 24.49      B
ATOM   3833  CB  PHE B 644      60.931  22.958  70.115  1.00 21.46      B
ATOM   3834  CG  PHE B 644      60.015  24.023  69.613  1.00 20.17      B
ATOM   3835  CD1 PHE B 644      59.720  24.125  68.258  1.00 22.46      B
ATOM   3836  CD2 PHE B 644      59.404  24.896  70.493  1.00 20.58      B
ATOM   3837  CE1 PHE B 644      58.816  25.079  67.783  1.00 20.21      B
ATOM   3838  CE2 PHE B 644      58.501  25.855  70.035  1.00 20.45      B
ATOM   3839  CZ  PHE B 644      58.207  25.942  68.674  1.00 20.84      B
ATOM   3840  C   PHE B 644      63.186  22.087  70.457  1.00 25.20      B
ATOM   3841  O   PHE B 644      63.886  21.534  69.613  1.00 24.80      B
ATOM   3842  N   LEU B 645      63.054  21.649  71.701  1.00 25.69      B
ATOM   3843  CA  LEU B 645      63.630  20.396  72.151  1.00 25.88      B
ATOM   3844  CB  LEU B 645      64.547  20.586  73.359  1.00 26.05      B
ATOM   3845  CG  LEU B 645      64.777  19.327  74.233  1.00 27.77      B
ATOM   3846  CD1 LEU B 645      66.044  18.602  73.852  1.00 28.34      B
ATOM   3847  CD2 LEU B 645      64.864  19.739  75.692  1.00 29.93      B
ATOM   3848  C   LEU B 645      62.349  19.704  72.590  1.00 26.32      B
ATOM   3849  O   LEU B 645      61.743  20.096  73.591  1.00 27.97      B
ATOM   3850  N   VAL B 646      61.910  18.706  71.834  1.00 25.54      B
ATOM   3851  CA  VAL B 646      60.688  18.005  72.191  1.00 25.91      B
ATOM   3852  CB  VAL B 646      59.892  17.651  70.918  1.00 25.69      B
ATOM   3853  CG1 VAL B 646      58.554  17.036  71.293  1.00 26.37      B
ATOM   3854  CG2 VAL B 646      59.681  18.909  70.069  1.00 23.92      B
ATOM   3855  C   VAL B 646      61.003  16.734  72.986  1.00 26.60      B
ATOM   3856  O   VAL B 646      62.051  16.130  72.780  1.00 27.76      B
ATOM   3857  N   SER B 647      60.121  16.358  73.916  1.00 27.17      B
ATOM   3858  CA  SER B 647      60.281  15.130  74.711  1.00 27.29      B
ATOM   3859  CB  SER B 647      60.956  15.417  76.054  1.00 27.08      B
ATOM   3860  OG  SER B 647      60.210  16.325  76.850  1.00 27.93      B
ATOM   3861  C   SER B 647      58.905  14.512  74.942  1.00 28.49      B
ATOM   3862  O   SER B 647      57.943  15.227  75.219  1.00 29.23      B
ATOM   3863  N   ALA B 648      58.819  13.189  74.800  1.00 28.67      B
ATOM   3864  CA  ALA B 648      57.568  12.454  74.976  1.00 28.62      B
ATOM   3865  CB  ALA B 648      57.093  11.906  73.630  1.00 28.17      B
ATOM   3866  C   ALA B 648      57.760  11.306  75.972  1.00 30.51      B
ATOM   3867  O   ALA B 648      58.756  10.577  75.898  1.00 31.42      B
ATOM   3868  N   ALA B 649      56.807  11.146  76.894  1.00 30.32      B
ATOM   3869  CA  ALA B 649      56.883  10.098  77.911  1.00 30.33      B
ATOM   3870  CB  ALA B 649      56.720  10.700  79.305  1.00 29.35      B
ATOM   3871  C   ALA B 649      55.863   8.988  77.711  1.00 31.09      B
ATOM   3872  O   ALA B 649      54.995   9.080  76.850  1.00 30.54      B
ATOM   3873  N   ALA B 650      55.981   7.941  78.530  1.00 32.95      B
ATOM   3874  CA  ALA B 650      55.103   6.768  78.483  1.00 32.69      B
ATOM   3875  CB  ALA B 650      55.783   5.597  79.194  1.00 30.66      B
ATOM   3876  C   ALA B 650      53.733   7.019  79.098  1.00 33.02      B
ATOM   3877  O   ALA B 650      52.941   6.091  79.251  1.00 32.69      B
ATOM   3878  N   ASP B 651      53.471   8.270  79.463  1.00 34.34      B
ATOM   3879  CA  ASP B 651      52.200   8.661  80.063  1.00 35.15      B
ATOM   3880  CB  ASP B 651      52.456   9.528  81.287  1.00 36.84      B
ATOM   3881  CG  ASP B 651      53.402  10.663  80.993  1.00 40.07      B
ATOM   3882  OD1 ASP B 651      53.652  10.935  79.800  1.00 40.99      B
ATOM   3883  OD2 ASP B 651      53.895  11.299  81.950  1.00 43.26      B
ATOM   3884  C   ASP B 651      51.347   9.441  79.068  1.00 35.49      B
ATOM   3885  O   ASP B 651      50.282   9.948  79.418  1.00 35.89      B
```

```
ATOM   3886  N   GLY B 652      51.833   9.542  77.834  1.00 34.99      B
ATOM   3887  CA  GLY B 652      51.110  10.260  76.802  1.00 34.08      B
ATOM   3888  C   GLY B 652      51.434  11.738  76.730  1.00 34.36      B
ATOM   3889  O   GLY B 652      50.877  12.449  75.891  1.00 36.08      B
ATOM   3890  N   SER B 653      52.336  12.198  77.595  1.00 32.03      B
ATOM   3891  CA  SER B 653      52.720  13.605  77.635  1.00 30.49      B
ATOM   3892  CB  SER B 653      53.176  13.995  79.050  1.00 31.53      B
ATOM   3893  OG  SER B 653      54.387  13.358  79.428  1.00 31.63      B
ATOM   3894  C   SER B 653      53.810  13.962  76.633  1.00 29.75      B
ATOM   3895  O   SER B 653      54.702  13.165  76.361  1.00 28.99      B
ATOM   3896  N   ILE B 654      53.733  15.175  76.097  1.00 30.15      B
ATOM   3897  CA  ILE B 654      54.703  15.655  75.115  1.00 30.00      B
ATOM   3898  CB  ILE B 654      54.083  15.708  73.706  1.00 29.09      B
ATOM   3899  CG2 ILE B 654      55.115  16.144  72.686  1.00 28.47      B
ATOM   3900  CG1 ILE B 654      53.548  14.336  73.318  1.00 28.15      B
ATOM   3901  CD1 ILE B 654      52.204  14.400  72.675  1.00 30.38      B
ATOM   3902  C   ILE B 654      55.109  17.061  75.508  1.00 30.87      B
ATOM   3903  O   ILE B 654      54.285  17.974  75.484  1.00 32.52      B
ATOM   3904  N   ARG B 655      56.371  17.241  75.878  1.00 30.22      B
ATOM   3905  CA  ARG B 655      56.835  18.570  76.271  1.00 29.48      B
ATOM   3906  CB  ARG B 655      57.614  18.492  77.589  1.00 31.26      B
ATOM   3907  CG  ARG B 655      56.773  18.219  78.827  1.00 34.00      B
ATOM   3908  CD  ARG B 655      56.140  19.500  79.287  1.00 40.70      B
ATOM   3909  NE  ARG B 655      55.601  19.484  80.657  1.00 45.23      B
ATOM   3910  CZ  ARG B 655      54.582  18.735  81.075  1.00 48.41      B
ATOM   3911  NH1 ARG B 655      53.979  17.909  80.234  1.00 49.81      B
ATOM   3912  NH2 ARG B 655      54.137  18.847  82.324  1.00 50.20      B
ATOM   3913  C   ARG B 655      57.712  19.195  75.187  1.00 28.14      B
ATOM   3914  O   ARG B 655      58.462  18.501  74.500  1.00 27.90      B
ATOM   3915  N   GLY B 656      57.582  20.507  75.033  1.00 26.00      B
ATOM   3916  CA  GLY B 656      58.365  21.237  74.065  1.00 24.28      B
ATOM   3917  C   GLY B 656      59.047  22.348  74.830  1.00 24.73      B
ATOM   3918  O   GLY B 656      58.384  23.228  75.386  1.00 26.11      B
ATOM   3919  N   TRP B 657      60.373  22.296  74.883  1.00 24.11      B
ATOM   3920  CA  TRP B 657      61.163  23.294  75.601  1.00 23.50      B
ATOM   3921  CB  TRP B 657      62.139  22.602  76.550  1.00 22.75      B
ATOM   3922  CG  TRP B 657      61.579  21.381  77.189  1.00 21.95      B
ATOM   3923  CD2 TRP B 657      61.213  21.230  78.562  1.00 19.79      B
ATOM   3924  CE2 TRP B 657      60.639  19.948  78.698  1.00 20.88      B
ATOM   3925  CE3 TRP B 657      61.320  22.048  79.691  1.00 19.86      B
ATOM   3926  CD1 TRP B 657      61.231  20.213  76.566  1.00 20.79      B
ATOM   3927  NE1 TRP B 657      60.657  19.350  77.469  1.00 20.21      B
ATOM   3928  CZ2 TRP B 657      60.160  19.478  79.926  1.00 21.49      B
ATOM   3929  CZ3 TRP B 657      60.846  21.570  80.915  1.00 20.44      B
ATOM   3930  CH2 TRP B 657      60.278  20.301  81.019  1.00 20.36      B
ATOM   3931  C   TRP B 657      61.966  24.122  74.610  1.00 24.96      B
ATOM   3932  O   TRP B 657      62.262  23.673  73.498  1.00 24.34      B
ATOM   3933  N   ASP B 658      62.331  25.331  75.014  1.00 26.03      B
ATOM   3934  CA  ASP B 658      63.126  26.181  74.137  1.00 28.03      B
ATOM   3935  CB  ASP B 658      63.307  27.565  74.741  1.00 28.12      B
ATOM   3936  CG  ASP B 658      64.031  28.494  73.805  1.00 29.75      B
ATOM   3937  OD1 ASP B 658      65.264  28.356  73.641  1.00 28.58      B
ATOM   3938  OD2 ASP B 658      63.352  29.351  73.209  1.00 31.24      B
ATOM   3939  C   ASP B 658      64.498  25.538  73.961  1.00 28.55      B
```

ATOM	3940	O	ASP	B	658	65.168	25.253	74.948	1.00	31.11	B
ATOM	3941	N	ALA	B	659	64.924	25.334	72.719	1.00	27.30	B
ATOM	3942	CA	ALA	B	659	66.209	24.689	72.443	1.00	28.28	B
ATOM	3943	CB	ALA	B	659	66.413	24.549	70.945	1.00	26.59	B
ATOM	3944	C	ALA	B	659	67.430	25.362	73.047	1.00	29.08	B
ATOM	3945	O	ALA	B	659	68.518	24.784	73.067	1.00	30.37	B
ATOM	3946	N	ASN	B	660	67.272	26.577	73.544	1.00	29.04	B
ATOM	3947	CA	ASN	B	660	68.419	27.256	74.090	1.00	29.15	B
ATOM	3948	CB	ASN	B	660	68.618	28.573	73.361	1.00	32.02	B
ATOM	3949	CG	ASN	B	660	69.953	29.185	73.646	1.00	36.15	B
ATOM	3950	OD1	ASN	B	660	70.999	28.600	73.342	1.00	39.04	B
ATOM	3951	ND2	ASN	B	660	69.939	30.371	74.238	1.00	38.31	B
ATOM	3952	C	ASN	B	660	68.334	27.474	75.582	1.00	28.96	B
ATOM	3953	O	ASN	B	660	69.262	27.138	76.301	1.00	30.76	B
ATOM	3954	N	ASP	B	661	67.225	28.024	76.059	1.00	28.20	B
ATOM	3955	CA	ASP	B	661	67.073	28.249	77.485	1.00	26.87	B
ATOM	3956	CB	ASP	B	661	66.553	29.663	77.745	1.00	29.19	B
ATOM	3957	CG	ASP	B	661	65.311	29.984	76.942	1.00	30.92	B
ATOM	3958	OD1	ASP	B	661	65.314	31.019	76.232	1.00	32.39	B
ATOM	3959	OD2	ASP	B	661	64.334	29.209	77.023	1.00	30.85	B
ATOM	3960	C	ASP	B	661	66.147	27.217	78.129	1.00	26.15	B
ATOM	3961	O	ASP	B	661	66.041	27.165	79.346	1.00	28.27	B
ATOM	3962	N	TYR	B	662	65.474	26.409	77.317	1.00	22.94	B
ATOM	3963	CA	TYR	B	662	64.590	25.365	77.819	1.00	21.57	B
ATOM	3964	CB	TYR	B	662	65.407	24.340	78.623	1.00	20.55	B
ATOM	3965	CG	TYR	B	662	66.647	23.879	77.871	1.00	21.52	B
ATOM	3966	CD1	TYR	B	662	67.867	24.533	78.019	1.00	19.76	B
ATOM	3967	CE1	TYR	B	662	68.960	24.193	77.231	1.00	18.58	B
ATOM	3968	CD2	TYR	B	662	66.567	22.861	76.919	1.00	20.80	B
ATOM	3969	CE2	TYR	B	662	67.659	22.519	76.126	1.00	18.36	B
ATOM	3970	CZ	TYR	B	662	68.851	23.192	76.287	1.00	18.65	B
ATOM	3971	OH	TYR	B	662	69.935	22.893	75.493	1.00	18.77	B
ATOM	3972	C	TYR	B	662	63.346	25.808	78.604	1.00	21.16	B
ATOM	3973	O	TYR	B	662	62.835	25.068	79.443	1.00	20.62	B
ATOM	3974	N	SER	B	663	62.864	27.015	78.327	1.00	21.52	B
ATOM	3975	CA	SER	B	663	61.642	27.500	78.954	1.00	21.24	B
ATOM	3976	CB	SER	B	663	61.458	28.993	78.699	1.00	19.14	B
ATOM	3977	OG	SER	B	663	61.441	29.273	77.312	1.00	19.19	B
ATOM	3978	C	SER	B	663	60.496	26.728	78.294	1.00	21.60	B
ATOM	3979	O	SER	B	663	60.585	26.352	77.123	1.00	20.87	B
ATOM	3980	N	ARG	B	664	59.436	26.489	79.057	1.00	22.75	B
ATOM	3981	CA	ARG	B	664	58.267	25.755	78.592	1.00	23.75	B
ATOM	3982	CB	ARG	B	664	57.317	25.544	79.764	1.00	26.18	B
ATOM	3983	CG	ARG	B	664	58.032	24.928	80.948	1.00	33.56	B
ATOM	3984	CD	ARG	B	664	57.130	24.061	81.812	1.00	39.29	B
ATOM	3985	NE	ARG	B	664	57.925	23.331	82.801	1.00	43.83	B
ATOM	3986	CZ	ARG	B	664	57.446	22.404	83.625	1.00	47.40	B
ATOM	3987	NH1	ARG	B	664	56.158	22.076	83.594	1.00	48.81	B
ATOM	3988	NH2	ARG	B	664	58.265	21.796	84.474	1.00	48.40	B
ATOM	3989	C	ARG	B	664	57.540	26.436	77.433	1.00	23.79	B
ATOM	3990	O	ARG	B	664	56.829	27.420	77.632	1.00	23.72	B
ATOM	3991	N	LYS	B	665	57.702	25.886	76.228	1.00	23.87	B
ATOM	3992	CA	LYS	B	665	57.091	26.453	75.021	1.00	24.18	B
ATOM	3993	CB	LYS	B	665	58.099	26.400	73.869	1.00	25.26	B

```
ATOM   3994  CG  LYS B 665      59.088  27.551  73.869  1.00 26.13      B
ATOM   3995  CD  LYS B 665      58.423  28.779  73.292  1.00 31.91      B
ATOM   3996  CE  LYS B 665      59.389  29.964  73.126  1.00 34.51      B
ATOM   3997  NZ  LYS B 665      59.804  30.608  74.426  1.00 40.98      B
ATOM   3998  C   LYS B 665      55.760  25.844  74.588  1.00 22.25      B
ATOM   3999  O   LYS B 665      54.943  26.514  73.956  1.00 21.84      B
ATOM   4000  N   PHE B 666      55.555  24.574  74.917  1.00 22.07      B
ATOM   4001  CA  PHE B 666      54.308  23.875  74.604  1.00 22.00      B
ATOM   4002  CB  PHE B 666      54.109  23.776  73.076  1.00 21.53      B
ATOM   4003  CG  PHE B 666      55.017  22.786  72.373  1.00 21.45      B
ATOM   4004  CD1 PHE B 666      54.744  21.420  72.408  1.00 21.12      B
ATOM   4005  CD2 PHE B 666      56.134  23.218  71.664  1.00 20.63      B
ATOM   4006  CE1 PHE B 666      55.562  20.506  71.758  1.00 17.08      B
ATOM   4007  CE2 PHE B 666      56.951  22.303  71.015  1.00 19.89      B
ATOM   4008  CZ  PHE B 666      56.659  20.947  71.066  1.00 17.19      B
ATOM   4009  C   PHE B 666      54.272  22.494  75.288  1.00 22.61      B
ATOM   4010  O   PHE B 666      55.323  21.938  75.618  1.00 24.01      B
ATOM   4011  N   SER B 667      53.068  21.973  75.538  1.00 22.74      B
ATOM   4012  CA  SER B 667      52.891  20.674  76.200  1.00 23.29      B
ATOM   4013  CB  SER B 667      52.827  20.831  77.717  1.00 22.23      B
ATOM   4014  OG  SER B 667      51.487  20.937  78.145  1.00 23.02      B
ATOM   4015  C   SER B 667      51.596  20.014  75.737  1.00 24.06      B
ATOM   4016  O   SER B 667      50.525  20.635  75.772  1.00 23.18      B
ATOM   4017  N   TYR B 668      51.703  18.751  75.321  1.00 24.19      B
ATOM   4018  CA  TYR B 668      50.554  17.999  74.834  1.00 24.45      B
ATOM   4019  CB  TYR B 668      50.633  17.810  73.324  1.00 24.25      B
ATOM   4020  CG  TYR B 668      50.638  19.089  72.543  1.00 24.38      B
ATOM   4021  CD1 TYR B 668      51.752  19.452  71.785  1.00 23.71      B
ATOM   4022  CE1 TYR B 668      51.759  20.610  71.024  1.00 24.24      B
ATOM   4023  CD2 TYR B 668      49.519  19.924  72.528  1.00 24.84      B
ATOM   4024  CE2 TYR B 668      49.514  21.091  71.770  1.00 25.84      B
ATOM   4025  CZ  TYR B 668      50.643  21.426  71.017  1.00 26.29      B
ATOM   4026  OH  TYR B 668      50.656  22.572  70.263  1.00 27.29      B
ATOM   4027  C   TYR B 668      50.391  16.634  75.462  1.00 23.76      B
ATOM   4028  O   TYR B 668      51.364  15.944  75.751  1.00 23.84      B
ATOM   4029  N   HIS B 669      49.144  16.223  75.612  1.00 24.21      B
ATOM   4030  CA  HIS B 669      48.864  14.948  76.225  1.00 26.26      B
ATOM   4031  CB  HIS B 669      48.329  15.214  77.623  1.00 27.79      B
ATOM   4032  CG  HIS B 669      48.682  14.159  78.607  1.00 30.20      B
ATOM   4033  CD2 HIS B 669      48.174  12.921  78.797  1.00 32.47      B
ATOM   4034  ND1 HIS B 669      49.695  14.309  79.526  1.00 30.16      B
ATOM   4035  CE1 HIS B 669      49.796  13.205  80.244  1.00 31.69      B
ATOM   4036  NE2 HIS B 669      48.884  12.347  79.822  1.00 32.65      B
ATOM   4037  C   HIS B 669      47.836  14.157  75.421  1.00 25.01      B
ATOM   4038  O   HIS B 669      46.743  14.662  75.167  1.00 25.41      B
ATOM   4039  N   HIS B 670      48.163  12.936  75.003  1.00 24.99      B
ATOM   4040  CA  HIS B 670      47.173  12.152  74.262  1.00 26.67      B
ATOM   4041  CB  HIS B 670      47.788  10.894  73.644  1.00 26.67      B
ATOM   4042  CG  HIS B 670      48.526  11.149  72.367  1.00 28.25      B
ATOM   4043  CD2 HIS B 670      49.149  12.266  71.911  1.00 27.02      B
ATOM   4044  ND1 HIS B 670      48.704  10.187  71.399  1.00 28.10      B
ATOM   4045  CE1 HIS B 670      49.404  10.697  70.398  1.00 27.39      B
ATOM   4046  NE2 HIS B 670      49.685  11.955  70.687  1.00 25.82      B
ATOM   4047  C   HIS B 670      46.033  11.766  75.198  1.00 28.34      B
```

```
ATOM   4048  O   HIS B 670      46.255  11.292  76.320  1.00 28.98      B
ATOM   4049  N   THR B 671      44.812  11.970  74.717  1.00 29.18      B
ATOM   4050  CA  THR B 671      43.597  11.706  75.479  1.00 29.09      B
ATOM   4051  CB  THR B 671      42.363  11.963  74.600  1.00 28.97      B
ATOM   4052  OG1 THR B 671      42.582  11.400  73.299  1.00 29.48      B
ATOM   4053  CG2 THR B 671      42.108  13.457  74.470  1.00 28.78      B
ATOM   4054  C   THR B 671      43.434  10.341  76.127  1.00 27.51      B
ATOM   4055  O   THR B 671      42.911  10.245  77.234  1.00 26.92      B
ATOM   4056  N   ASN B 672      43.857   9.291  75.436  1.00 28.14      B
ATOM   4057  CA  ASN B 672      43.715   7.936  75.961  1.00 29.14      B
ATOM   4058  CB  ASN B 672      43.528   6.943  74.808  1.00 30.07      B
ATOM   4059  CG  ASN B 672      44.774   6.802  73.954  1.00 31.70      B
ATOM   4060  OD1 ASN B 672      45.721   7.592  74.082  1.00 32.55      B
ATOM   4061  ND2 ASN B 672      44.779   5.803  73.067  1.00 30.68      B
ATOM   4062  C   ASN B 672      44.911   7.538  76.819  1.00 27.80      B
ATOM   4063  O   ASN B 672      45.184   6.354  77.040  1.00 25.74      B
ATOM   4064  N   LEU B 673      45.624   8.554  77.283  1.00 27.49      B
ATOM   4065  CA  LEU B 673      46.771   8.370  78.152  1.00 28.57      B
ATOM   4066  CB  LEU B 673      46.267   8.132  79.581  1.00 26.43      B
ATOM   4067  CG  LEU B 673      45.295   9.183  80.132  1.00 27.88      B
ATOM   4068  CD1 LEU B 673      44.949   8.826  81.572  1.00 28.51      B
ATOM   4069  CD2 LEU B 673      45.898  10.581  80.067  1.00 26.47      B
ATOM   4070  C   LEU B 673      47.711   7.243  77.727  1.00 28.78      B
ATOM   4071  O   LEU B 673      48.353   6.613  78.560  1.00 28.06      B
ATOM   4072  N   SER B 674      47.805   6.992  76.431  1.00 29.36      B
ATOM   4073  CA  SER B 674      48.676   5.926  75.960  1.00 29.70      B
ATOM   4074  CB  SER B 674      48.207   5.459  74.585  1.00 32.41      B
ATOM   4075  OG  SER B 674      46.859   5.039  74.652  1.00 35.35      B
ATOM   4076  C   SER B 674      50.140   6.353  75.892  1.00 27.54      B
ATOM   4077  O   SER B 674      50.438   7.522  75.678  1.00 27.24      B
ATOM   4078  N   ALA B 675      51.053   5.407  76.074  1.00 25.24      B
ATOM   4079  CA  ALA B 675      52.455   5.748  76.006  1.00 24.53      B
ATOM   4080  CB  ALA B 675      53.304   4.573  76.393  1.00 25.14      B
ATOM   4081  C   ALA B 675      52.793   6.179  74.589  1.00 25.51      B
ATOM   4082  O   ALA B 675      52.484   5.472  73.610  1.00 26.90      B
ATOM   4083  N   ILE B 676      53.429   7.340  74.485  1.00 23.80      B
ATOM   4084  CA  ILE B 676      53.824   7.880  73.200  1.00 23.18      B
ATOM   4085  CB  ILE B 676      54.457   9.276  73.354  1.00 22.28      B
ATOM   4086  CG2 ILE B 676      54.960   9.749  71.999  1.00 26.37      B
ATOM   4087  CG1 ILE B 676      53.437  10.265  73.913  1.00 20.36      B
ATOM   4088  CD1 ILE B 676      52.158  10.388  73.112  1.00 19.30      B
ATOM   4089  C   ILE B 676      54.835   6.966  72.505  1.00 23.03      B
ATOM   4090  O   ILE B 676      55.939   6.770  73.005  1.00 22.66      B
ATOM   4091  N   THR B 677      54.454   6.432  71.344  1.00 23.91      B
ATOM   4092  CA  THR B 677      55.310   5.536  70.554  1.00 24.45      B
ATOM   4093  CB  THR B 677      54.495   4.625  69.663  1.00 21.85      B
ATOM   4094  OG1 THR B 677      53.512   3.966  70.447  1.00 21.96      B
ATOM   4095  CG2 THR B 677      55.406   3.590  69.020  1.00 27.86      B
ATOM   4096  C   THR B 677      56.291   6.286  69.642  1.00 26.36      B
ATOM   4097  O   THR B 677      57.469   5.953  69.580  1.00 26.98      B
ATOM   4098  N   THR B 678      55.787   7.252  68.884  1.00 27.47      B
ATOM   4099  CA  THR B 678      56.647   8.070  68.046  1.00 28.85      B
ATOM   4100  CB  THR B 678      56.939   7.483  66.615  1.00 31.08      B
ATOM   4101  OG1 THR B 678      55.731   7.007  66.003  1.00 33.29      B
```

```
ATOM   4102  CG2 THR B 678      57.971   6.378  66.698  1.00 35.12      B
ATOM   4103  C   THR B 678      56.070   9.447  67.831  1.00 28.29      B
ATOM   4104  O   THR B 678      54.934   9.742  68.215  1.00 29.19      B
ATOM   4105  N   PHE B 679      56.889  10.273  67.194  1.00 27.12      B
ATOM   4106  CA  PHE B 679      56.552  11.621  66.835  1.00 24.71      B
ATOM   4107  CB  PHE B 679      56.246  12.453  68.085  1.00 25.37      B
ATOM   4108  CG  PHE B 679      57.481  12.945  68.829  1.00 24.77      B
ATOM   4109  CD1 PHE B 679      58.206  14.061  68.374  1.00 21.98      B
ATOM   4110  CD2 PHE B 679      57.916  12.293  69.990  1.00 24.36      B
ATOM   4111  CE1 PHE B 679      59.331  14.509  69.063  1.00 19.92      B
ATOM   4112  CE2 PHE B 679      59.032  12.736  70.671  1.00 22.18      B
ATOM   4113  CZ  PHE B 679      59.739  13.845  70.207  1.00 21.94      B
ATOM   4114  C   PHE B 679      57.762  12.174  66.095  1.00 24.89      B
ATOM   4115  O   PHE B 679      58.894  11.669  66.212  1.00 21.91      B
ATOM   4116  N   TYR B 680      57.504  13.231  65.338  1.00 25.98      B
ATOM   4117  CA  TYR B 680      58.516  13.918  64.557  1.00 25.00      B
ATOM   4118  CB  TYR B 680      58.418  13.438  63.104  1.00 23.81      B
ATOM   4119  CG  TYR B 680      59.668  13.711  62.317  1.00 27.68      B
ATOM   4120  CD1 TYR B 680      60.795  12.881  62.429  1.00 26.50      B
ATOM   4121  CE1 TYR B 680      62.003  13.232  61.812  1.00 27.92      B
ATOM   4122  CD2 TYR B 680      59.780  14.881  61.559  1.00 28.23      B
ATOM   4123  CE2 TYR B 680      60.971  15.237  60.949  1.00 27.91      B
ATOM   4124  CZ  TYR B 680      62.074  14.427  61.080  1.00 28.40      B
ATOM   4125  OH  TYR B 680      63.253  14.870  60.531  1.00 31.86      B
ATOM   4126  C   TYR B 680      58.122  15.405  64.735  1.00 23.73      B
ATOM   4127  O   TYR B 680      56.975  15.684  65.090  1.00 22.88      B
ATOM   4128  N   VAL B 681      59.053  16.340  64.520  1.00 23.01      B
ATOM   4129  CA  VAL B 681      58.785  17.781  64.698  1.00 21.87      B
ATOM   4130  CB  VAL B 681      59.211  18.315  66.071  1.00 20.14      B
ATOM   4131  CG1 VAL B 681      58.030  18.505  66.979  1.00 18.83      B
ATOM   4132  CG2 VAL B 681      60.254  17.397  66.641  1.00 21.44      B
ATOM   4133  C   VAL B 681      59.556  18.695  63.781  1.00 21.58      B
ATOM   4134  O   VAL B 681      60.694  18.427  63.399  1.00 19.29      B
ATOM   4135  N   SER B 682      58.928  19.818  63.480  1.00 21.27      B
ATOM   4136  CA  SER B 682      59.554  20.864  62.685  1.00 20.48      B
ATOM   4137  CB  SER B 682      58.923  20.956  61.300  1.00 19.96      B
ATOM   4138  OG  SER B 682      57.535  21.230  61.396  1.00 20.38      B
ATOM   4139  C   SER B 682      59.174  22.065  63.518  1.00 20.44      B
ATOM   4140  O   SER B 682      58.332  21.944  64.407  1.00 22.67      B
ATOM   4141  N   ASP B 683      59.797  23.207  63.275  1.00 19.98      B
ATOM   4142  CA  ASP B 683      59.441  24.394  64.036  1.00 19.73      B
ATOM   4143  CB  ASP B 683      60.212  25.638  63.547  1.00 20.26      B
ATOM   4144  CG  ASP B 683      61.708  25.650  63.959  1.00 21.54      B
ATOM   4145  OD1 ASP B 683      62.132  24.891  64.860  1.00 19.41      B
ATOM   4146  OD2 ASP B 683      62.468  26.460  63.377  1.00 22.23      B
ATOM   4147  C   ASP B 683      57.936  24.665  63.889  1.00 18.98      B
ATOM   4148  O   ASP B 683      57.351  25.254  64.782  1.00 19.03      B
ATOM   4149  N   ASN B 684      57.311  24.214  62.800  1.00 18.67      B
ATOM   4150  CA  ASN B 684      55.888  24.482  62.579  1.00 20.77      B
ATOM   4151  CB  ASN B 684      55.644  24.891  61.136  1.00 20.60      B
ATOM   4152  CG  ASN B 684      56.303  26.196  60.780  1.00 23.83      B
ATOM   4153  OD1 ASN B 684      56.062  27.233  61.419  1.00 24.57      B
ATOM   4154  ND2 ASN B 684      57.134  26.165  59.741  1.00 23.71      B
ATOM   4155  C   ASN B 684      54.874  23.392  62.886  1.00 22.90      B
```

```
ATOM   4156  O   ASN B 684      53.687  23.690  63.077  1.00 22.24      B
ATOM   4157  N   ILE B 685      55.327  22.140  62.890  1.00 23.24      B
ATOM   4158  CA  ILE B 685      54.449  20.997  63.118  1.00 20.82      B
ATOM   4159  CB  ILE B 685      54.156  20.257  61.778  1.00 19.24      B
ATOM   4160  CG2 ILE B 685      53.256  19.057  62.014  1.00 18.99      B
ATOM   4161  CG1 ILE B 685      53.488  21.211  60.784  1.00 17.58      B
ATOM   4162  CD1 ILE B 685      52.067  21.562  61.120  1.00 17.99      B
ATOM   4163  C   ILE B 685      55.037  19.993  64.100  1.00 21.40      B
ATOM   4164  O   ILE B 685      56.263  19.961  64.315  1.00 21.31      B
ATOM   4165  N   LEU B 686      54.137  19.207  64.697  1.00 20.50      B
ATOM   4166  CA  LEU B 686      54.461  18.147  65.648  1.00 21.98      B
ATOM   4167  CB  LEU B 686      54.273  18.612  67.108  1.00 23.37      B
ATOM   4168  CG  LEU B 686      54.138  17.518  68.189  1.00 24.30      B
ATOM   4169  CD1 LEU B 686      55.479  16.866  68.430  1.00 24.15      B
ATOM   4170  CD2 LEU B 686      53.595  18.098  69.475  1.00 22.84      B
ATOM   4171  C   LEU B 686      53.475  17.026  65.361  1.00 22.92      B
ATOM   4172  O   LEU B 686      52.297  17.167  65.650  1.00 25.29      B
ATOM   4173  N   VAL B 687      53.927  15.924  64.780  1.00 21.99      B
ATOM   4174  CA  VAL B 687      53.018  14.817  64.511  1.00 21.64      B
ATOM   4175  CB  VAL B 687      53.186  14.346  63.000  1.00 22.41      B
ATOM   4176  CG1 VAL B 687      52.604  12.949  62.796  1.00 21.78      B
ATOM   4177  CG2 VAL B 687      52.476  15.325  62.052  1.00 19.88      B
ATOM   4178  C   VAL B 687      53.345  13.700  65.542  1.00 21.43      B
ATOM   4179  O   VAL B 687      54.476  13.202  65.599  1.00 21.65      B
ATOM   4180  N   SER B 688      52.387  13.330  66.390  1.00 21.20      B
ATOM   4181  CA  SER B 688      52.654  12.302  67.412  1.00 21.07      B
ATOM   4182  CB  SER B 688      52.601  12.920  68.812  1.00 21.19      B
ATOM   4183  OG  SER B 688      51.336  13.509  69.074  1.00 19.67      B
ATOM   4184  C   SER B 688      51.706  11.118  67.373  1.00 21.57      B
ATOM   4185  O   SER B 688      50.511  11.265  67.104  1.00 21.58      B
ATOM   4186  N   GLY B 689      52.221   9.935  67.674  1.00 23.31      B
ATOM   4187  CA  GLY B 689      51.348   8.778  67.635  1.00 25.20      B
ATOM   4188  C   GLY B 689      51.498   7.793  68.779  1.00 26.22      B
ATOM   4189  O   GLY B 689      52.590   7.549  69.295  1.00 26.74      B
ATOM   4190  N   SER B 690      50.372   7.245  69.200  1.00 26.47      B
ATOM   4191  CA  SER B 690      50.350   6.247  70.253  1.00 29.04      B
ATOM   4192  CB  SER B 690      49.977   6.881  71.601  1.00 30.51      B
ATOM   4193  OG  SER B 690      48.577   7.150  71.674  1.00 31.85      B
ATOM   4194  C   SER B 690      49.261   5.262  69.818  1.00 29.64      B
ATOM   4195  O   SER B 690      48.624   5.462  68.788  1.00 31.71      B
ATOM   4196  N   GLU B 691      49.037   4.213  70.599  1.00 29.52      B
ATOM   4197  CA  GLU B 691      48.005   3.239  70.280  1.00 28.36      B
ATOM   4198  CB  GLU B 691      47.857   2.282  71.452  1.00 28.07      B
ATOM   4199  CG  GLU B 691      46.563   1.512  71.496  1.00 32.75      B
ATOM   4200  CD  GLU B 691      46.531   0.499  72.635  1.00 35.90      B
ATOM   4201  OE1 GLU B 691      47.285  -0.507  72.575  1.00 37.07      B
ATOM   4202  OE2 GLU B 691      45.751   0.712  73.594  1.00 36.72      B
ATOM   4203  C   GLU B 691      46.689   3.970  70.013  1.00 27.98      B
ATOM   4204  O   GLU B 691      46.356   4.921  70.713  1.00 29.12      B
ATOM   4205  N   ASN B 692      45.968   3.554  68.974  1.00 27.34      B
ATOM   4206  CA  ASN B 692      44.678   4.159  68.617  1.00 27.55      B
ATOM   4207  CB  ASN B 692      43.625   3.832  69.671  1.00 30.51      B
ATOM   4208  CG  ASN B 692      43.363   2.347  69.797  1.00 33.53      B
ATOM   4209  OD1 ASN B 692      42.997   1.866  70.874  1.00 34.93      B
```

```
ATOM   4210  ND2 ASN B 692      43.537   1.607  68.694  1.00 36.41      B
ATOM   4211  C   ASN B 692      44.671   5.671  68.417  1.00 28.06      B
ATOM   4212  O   ASN B 692      43.611   6.271  68.227  1.00 27.85      B
ATOM   4213  N   GLN B 693      45.836   6.300  68.455  1.00 27.40      B
ATOM   4214  CA  GLN B 693      45.883   7.737  68.270  1.00 26.47      B
ATOM   4215  CB  GLN B 693      46.046   8.410  69.627  1.00 26.45      B
ATOM   4216  CG  GLN B 693      44.860   8.235  70.547  1.00 27.10      B
ATOM   4217  CD  GLN B 693      44.499   9.523  71.245  1.00 27.21      B
ATOM   4218  OE1 GLN B 693      45.360  10.211  71.776  1.00 28.92      B
ATOM   4219  NE2 GLN B 693      43.224   9.859  71.243  1.00 29.30      B
ATOM   4220  C   GLN B 693      46.999   8.200  67.320  1.00 26.29      B
ATOM   4221  O   GLN B 693      48.105   7.655  67.332  1.00 27.55      B
ATOM   4222  N   PHE B 694      46.700   9.196  66.487  1.00 24.60      B
ATOM   4223  CA  PHE B 694      47.675   9.771  65.551  1.00 22.51      B
ATOM   4224  CB  PHE B 694      47.612   9.073  64.184  1.00 20.48      B
ATOM   4225  CG  PHE B 694      48.701   9.499  63.210  1.00 20.42      B
ATOM   4226  CD1 PHE B 694      49.967   8.922  63.241  1.00 20.85      B
ATOM   4227  CD2 PHE B 694      48.441  10.465  62.237  1.00 21.71      B
ATOM   4228  CE1 PHE B 694      50.956   9.301  62.312  1.00 21.35      B
ATOM   4229  CE2 PHE B 694      49.421  10.851  61.304  1.00 20.94      B
ATOM   4230  CZ  PHE B 694      50.674  10.269  61.343  1.00 20.97      B
ATOM   4231  C   PHE B 694      47.234  11.227  65.445  1.00 22.04      B
ATOM   4232  O   PHE B 694      46.146  11.508  64.951  1.00 22.64      B
ATOM   4233  N   ASN B 695      48.065  12.142  65.947  1.00 22.40      B
ATOM   4234  CA  ASN B 695      47.741  13.570  65.946  1.00 22.71      B
ATOM   4235  CB  ASN B 695      47.542  14.102  67.383  1.00 24.16      B
ATOM   4236  CG  ASN B 695      46.687  13.194  68.246  1.00 27.03      B
ATOM   4237  OD1 ASN B 695      47.145  12.735  69.297  1.00 30.17      B
ATOM   4238  ND2 ASN B 695      45.441  12.930  67.817  1.00 28.07      B
ATOM   4239  C   ASN B 695      48.762  14.477  65.261  1.00 21.75      B
ATOM   4240  O   ASN B 695      49.960  14.194  65.232  1.00 20.80      B
ATOM   4241  N   ILE B 696      48.248  15.588  64.734  1.00 21.52      B
ATOM   4242  CA  ILE B 696      49.024  16.622  64.045  1.00 20.16      B
ATOM   4243  CB  ILE B 696      48.592  16.711  62.556  1.00 17.92      B
ATOM   4244  CG2 ILE B 696      49.367  17.768  61.821  1.00 16.21      B
ATOM   4245  CG1 ILE B 696      48.860  15.371  61.883  1.00 16.96      B
ATOM   4246  CD1 ILE B 696      48.335  15.277  60.471  1.00 14.78      B
ATOM   4247  C   ILE B 696      48.732  17.922  64.803  1.00 20.71      B
ATOM   4248  O   ILE B 696      47.589  18.207  65.167  1.00 20.57      B
ATOM   4249  N   TYR B 697      49.779  18.690  65.057  1.00 21.04      B
ATOM   4250  CA  TYR B 697      49.651  19.916  65.816  1.00 22.01      B
ATOM   4251  CB  TYR B 697      50.334  19.746  67.174  1.00 22.18      B
ATOM   4252  CG  TYR B 697      49.748  18.654  68.027  1.00 22.67      B
ATOM   4253  CD1 TYR B 697      48.702  18.919  68.917  1.00 21.46      B
ATOM   4254  CE1 TYR B 697      48.167  17.910  69.717  1.00 20.34      B
ATOM   4255  CD2 TYR B 697      50.244  17.349  67.952  1.00 22.41      B
ATOM   4256  CE2 TYR B 697      49.717  16.331  68.746  1.00 22.87      B
ATOM   4257  CZ  TYR B 697      48.685  16.615  69.627  1.00 21.85      B
ATOM   4258  OH  TYR B 697      48.212  15.607  70.431  1.00 22.33      B
ATOM   4259  C   TYR B 697      50.244  21.121  65.112  1.00 23.61      B
ATOM   4260  O   TYR B 697      51.334  21.080  64.538  1.00 25.65      B
ATOM   4261  N   ASN B 698      49.491  22.202  65.162  1.00 23.81      B
ATOM   4262  CA  ASN B 698      49.913  23.449  64.594  1.00 23.42      B
ATOM   4263  CB  ASN B 698      48.680  24.254  64.224  1.00 26.51      B
```

```
ATOM   4264  CG  ASN B 698      49.020  25.531  63.512  1.00 28.61      B
ATOM   4265  OD1 ASN B 698      49.959  26.238  63.897  1.00 28.06      B
ATOM   4266  ND2 ASN B 698      48.255  25.849  62.472  1.00 29.88      B
ATOM   4267  C   ASN B 698      50.658  24.079  65.778  1.00 23.71      B
ATOM   4268  O   ASN B 698      50.047  24.586  66.726  1.00 22.24      B
ATOM   4269  N   LEU B 699      51.980  23.982  65.732  1.00 23.60      B
ATOM   4270  CA  LEU B 699      52.841  24.497  66.773  1.00 24.06      B
ATOM   4271  CB  LEU B 699      54.270  24.037  66.517  1.00 22.91      B
ATOM   4272  CG  LEU B 699      54.837  22.996  67.475  1.00 23.91      B
ATOM   4273  CD1 LEU B 699      53.784  21.972  67.874  1.00 24.32      B
ATOM   4274  CD2 LEU B 699      56.028  22.362  66.832  1.00 22.79      B
ATOM   4275  C   LEU B 699      52.801  26.001  66.862  1.00 25.53      B
ATOM   4276  O   LEU B 699      53.498  26.580  67.681  1.00 27.08      B
ATOM   4277  N   ARG B 700      52.004  26.631  66.002  1.00 26.51      B
ATOM   4278  CA  ARG B 700      51.863  28.087  65.997  1.00 25.40      B
ATOM   4279  CB  ARG B 700      51.489  28.600  64.609  1.00 27.54      B
ATOM   4280  CG  ARG B 700      52.549  28.502  63.543  1.00 28.72      B
ATOM   4281  CD  ARG B 700      53.706  29.422  63.820  1.00 31.33      B
ATOM   4282  NE  ARG B 700      54.598  29.480  62.671  1.00 34.27      B
ATOM   4283  CZ  ARG B 700      54.233  29.908  61.464  1.00 36.22      B
ATOM   4284  NH1 ARG B 700      52.989  30.318  61.259  1.00 35.49      B
ATOM   4285  NH2 ARG B 700      55.107  29.920  60.457  1.00 38.36      B
ATOM   4286  C   ARG B 700      50.724  28.431  66.942  1.00 24.24      B
ATOM   4287  O   ARG B 700      50.914  29.118  67.928  1.00 22.77      B
ATOM   4288  N   SER B 701      49.532  27.949  66.620  1.00 23.91      B
ATOM   4289  CA  SER B 701      48.358  28.202  67.435  1.00 23.69      B
ATOM   4290  CB  SER B 701      47.105  27.928  66.633  1.00 21.95      B
ATOM   4291  OG  SER B 701      47.096  26.574  66.220  1.00 21.41      B
ATOM   4292  C   SER B 701      48.342  27.281  68.627  1.00 25.56      B
ATOM   4293  O   SER B 701      47.546  27.467  69.541  1.00 27.95      B
ATOM   4294  N   GLY B 702      49.207  26.273  68.606  1.00 25.80      B
ATOM   4295  CA  GLY B 702      49.252  25.311  69.688  1.00 25.16      B
ATOM   4296  C   GLY B 702      48.080  24.351  69.601  1.00 25.57      B
ATOM   4297  O   GLY B 702      47.963  23.464  70.427  1.00 27.20      B
ATOM   4298  N   LYS B 703      47.221  24.498  68.597  1.00 26.86      B
ATOM   4299  CA  LYS B 703      46.049  23.630  68.485  1.00 29.85      B
ATOM   4300  CB  LYS B 703      44.846  24.452  67.982  1.00 31.50      B
ATOM   4301  CG  LYS B 703      44.521  25.679  68.857  1.00 35.32      B
ATOM   4302  CD  LYS B 703      43.066  26.160  68.704  1.00 35.78      B
ATOM   4303  CE  LYS B 703      42.529  26.768  70.007  1.00 39.24      B
ATOM   4304  NZ  LYS B 703      42.643  25.841  71.218  1.00 39.02      B
ATOM   4305  C   LYS B 703      46.199  22.357  67.631  1.00 29.87      B
ATOM   4306  O   LYS B 703      47.079  22.245  66.786  1.00 31.67      B
ATOM   4307  N   LEU B 704      45.314  21.403  67.868  1.00 29.38      B
ATOM   4308  CA  LEU B 704      45.319  20.152  67.149  1.00 29.31      B
ATOM   4309  CB  LEU B 704      44.445  19.169  67.892  1.00 28.56      B
ATOM   4310  CG  LEU B 704      44.409  17.731  67.419  1.00 29.17      B
ATOM   4311  CD1 LEU B 704      45.768  17.030  67.620  1.00 29.83      B
ATOM   4312  CD2 LEU B 704      43.340  17.041  68.206  1.00 28.68      B
ATOM   4313  C   LEU B 704      44.732  20.390  65.772  1.00 30.18      B
ATOM   4314  O   LEU B 704      43.610  20.880  65.669  1.00 32.27      B
ATOM   4315  N   VAL B 705      45.458  20.053  64.709  1.00 30.79      B
ATOM   4316  CA  VAL B 705      44.908  20.275  63.371  1.00 31.43      B
ATOM   4317  CB  VAL B 705      46.012  20.551  62.322  1.00 30.01      B
```

```
ATOM   4318  CG1 VAL B 705      45.368  20.883  60.976  1.00 28.32      B
ATOM   4319  CG2 VAL B 705      46.889  21.685  62.776  1.00 29.54      B
ATOM   4320  C   VAL B 705      44.069  19.087  62.904  1.00 32.61      B
ATOM   4321  O   VAL B 705      42.930  19.252  62.462  1.00 32.10      B
ATOM   4322  N   HIS B 706      44.641  17.890  63.003  1.00 35.60      B
ATOM   4323  CA  HIS B 706      43.949  16.665  62.613  1.00 37.51      B
ATOM   4324  CB  HIS B 706      44.515  16.131  61.302  1.00 40.51      B
ATOM   4325  CG  HIS B 706      44.191  16.972  60.110  1.00 43.09      B
ATOM   4326  CD2 HIS B 706      44.947  17.845  59.402  1.00 44.48      B
ATOM   4327  ND1 HIS B 706      42.946  16.973  59.521  1.00 43.58      B
ATOM   4328  CE1 HIS B 706      42.948  17.814  58.501  1.00 44.83      B
ATOM   4329  NE2 HIS B 706      44.149  18.357  58.407  1.00 45.93      B
ATOM   4330  C   HIS B 706      44.109  15.583  63.676  1.00 37.67      B
ATOM   4331  O   HIS B 706      45.189  15.396  64.267  1.00 38.10      B
ATOM   4332  N   ALA B 707      43.032  14.852  63.917  1.00 37.33      B
ATOM   4333  CA  ALA B 707      43.104  13.773  64.891  1.00 35.31      B
ATOM   4334  CB  ALA B 707      42.368  14.163  66.163  1.00 33.61      B
ATOM   4335  C   ALA B 707      42.540  12.479  64.322  1.00 33.93      B
ATOM   4336  O   ALA B 707      42.616  11.455  64.979  1.00 33.97      B
ATOM   4337  N   ASN B 708      42.000  12.508  63.103  1.00 32.93      B
ATOM   4338  CA  ASN B 708      41.438  11.278  62.566  1.00 32.08      B
ATOM   4339  CB  ASN B 708      39.900  11.381  62.527  1.00 30.21      B
ATOM   4340  CG  ASN B 708      39.282  11.431  63.935  1.00 29.73      B
ATOM   4341  OD1 ASN B 708      39.641  10.644  64.808  1.00 32.17      B
ATOM   4342  ND2 ASN B 708      38.369  12.355  64.155  1.00 27.91      B
ATOM   4343  C   ASN B 708      41.998  10.810  61.227  1.00 31.64      B
ATOM   4344  O   ASN B 708      41.468   9.888  60.605  1.00 30.96      B
ATOM   4345  N   ILE B 709      43.104  11.412  60.803  1.00 31.19      B
ATOM   4346  CA  ILE B 709      43.709  11.050  59.526  1.00 29.76      B
ATOM   4347  CB  ILE B 709      45.027  11.813  59.279  1.00 30.79      B
ATOM   4348  CG2 ILE B 709      45.414  11.698  57.830  1.00 30.87      B
ATOM   4349  CG1 ILE B 709      44.846  13.292  59.585  1.00 31.89      B
ATOM   4350  CD1 ILE B 709      43.831  13.966  58.690  1.00 33.84      B
ATOM   4351  C   ILE B 709      43.992   9.554  59.404  1.00 27.56      B
ATOM   4352  O   ILE B 709      43.923   9.003  58.316  1.00 28.85      B
ATOM   4353  N   LEU B 710      44.335   8.892  60.498  1.00 24.88      B
ATOM   4354  CA  LEU B 710      44.600   7.464  60.406  1.00 23.14      B
ATOM   4355  CB  LEU B 710      46.101   7.207  60.581  1.00 19.23      B
ATOM   4356  CG  LEU B 710      47.171   7.770  59.617  1.00 17.21      B
ATOM   4357  CD1 LEU B 710      48.565   7.336  60.119  1.00 12.65      B
ATOM   4358  CD2 LEU B 710      46.952   7.271  58.159  1.00 11.32      B
ATOM   4359  C   LEU B 710      43.787   6.738  61.491  1.00 24.82      B
ATOM   4360  O   LEU B 710      44.278   5.820  62.165  1.00 26.12      B
ATOM   4361  N   LYS B 711      42.540   7.172  61.668  1.00 24.22      B
ATOM   4362  CA  LYS B 711      41.672   6.583  62.678  1.00 23.87      B
ATOM   4363  CB  LYS B 711      40.223   7.113  62.551  1.00 23.07      B
ATOM   4364  CG  LYS B 711      39.704   7.286  61.127  0.00 24.07      B
ATOM   4365  CD  LYS B 711      39.138   6.000  60.567  0.00 24.51      B
ATOM   4366  CE  LYS B 711      38.815   6.171  59.096  0.00 24.91      B
ATOM   4367  NZ  LYS B 711      38.073   5.005  58.557  0.00 25.25      B
ATOM   4368  C   LYS B 711      41.697   5.066  62.640  1.00 22.54      B
ATOM   4369  O   LYS B 711      41.789   4.435  63.682  1.00 21.78      B
ATOM   4370  N   ASP B 712      41.656   4.474  61.450  1.00 24.59      B
ATOM   4371  CA  ASP B 712      41.649   3.009  61.346  1.00 26.66      B
```

```
ATOM   4372  CB  ASP B 712      41.358   2.577  59.902  1.00 27.40      B
ATOM   4373  CG  ASP B 712      42.533   2.779  58.971  1.00 29.97      B
ATOM   4374  OD1 ASP B 712      43.376   3.660  59.238  1.00 31.04      B
ATOM   4375  OD2 ASP B 712      42.601   2.059  57.945  1.00 32.95      B
ATOM   4376  C   ASP B 712      42.908   2.320  61.846  1.00 27.18      B
ATOM   4377  O   ASP B 712      42.933   1.100  61.992  1.00 28.41      B
ATOM   4378  N   ALA B 713      43.943   3.099  62.131  1.00 26.51      B
ATOM   4379  CA  ALA B 713      45.192   2.526  62.600  1.00 27.91      B
ATOM   4380  CB  ALA B 713      46.334   3.505  62.337  1.00 25.17      B
ATOM   4381  C   ALA B 713      45.117   2.185  64.091  1.00 29.57      B
ATOM   4382  O   ALA B 713      44.650   3.003  64.889  1.00 30.09      B
ATOM   4383  N   ASP B 714      45.584   0.991  64.467  1.00 30.92      B
ATOM   4384  CA  ASP B 714      45.568   0.564  65.873  1.00 33.02      B
ATOM   4385  CB  ASP B 714      45.300  -0.947  65.975  1.00 34.69      B
ATOM   4386  CG  ASP B 714      43.997  -1.348  65.333  1.00 36.43      B
ATOM   4387  OD1 ASP B 714      42.933  -0.920  65.810  1.00 38.16      B
ATOM   4388  OD2 ASP B 714      44.033  -2.089  64.337  1.00 40.68      B
ATOM   4389  C   ASP B 714      46.871   0.908  66.620  1.00 33.35      B
ATOM   4390  O   ASP B 714      46.871   1.124  67.837  1.00 33.65      B
ATOM   4391  N   GLN B 715      47.979   0.948  65.888  1.00 32.50      B
ATOM   4392  CA  GLN B 715      49.272   1.292  66.470  1.00 31.33      B
ATOM   4393  CB  GLN B 715      50.053   0.028  66.851  1.00 32.90      B
ATOM   4394  CG  GLN B 715      49.555  -0.657  68.107  1.00 36.42      B
ATOM   4395  CD  GLN B 715      49.806   0.172  69.355  1.00 39.19      B
ATOM   4396  OE1 GLN B 715      49.528  -0.273  70.465  1.00 39.45      B
ATOM   4397  NE2 GLN B 715      50.342   1.389  69.175  1.00 41.12      B
ATOM   4398  C   GLN B 715      50.063   2.123  65.465  1.00 29.87      B
ATOM   4399  O   GLN B 715      49.897   1.967  64.254  1.00 28.89      B
ATOM   4400  N   ILE B 716      50.885   3.038  65.968  1.00 28.35      B
ATOM   4401  CA  ILE B 716      51.712   3.875  65.102  1.00 26.58      B
ATOM   4402  CB  ILE B 716      51.360   5.388  65.216  1.00 26.71      B
ATOM   4403  CG2 ILE B 716      52.387   6.226  64.452  1.00 24.23      B
ATOM   4404  CG1 ILE B 716      49.979   5.655  64.611  1.00 27.09      B
ATOM   4405  CD1 ILE B 716      48.830   5.042  65.381  1.00 29.06      B
ATOM   4406  C   ILE B 716      53.137   3.644  65.567  1.00 26.24      B
ATOM   4407  O   ILE B 716      53.563   4.184  66.583  1.00 25.69      B
ATOM   4408  N   TRP B 717      53.870   2.833  64.818  1.00 25.09      B
ATOM   4409  CA  TRP B 717      55.219   2.505  65.198  1.00 25.49      B
ATOM   4410  CB  TRP B 717      55.658   1.210  64.497  1.00 28.30      B
ATOM   4411  CG  TRP B 717      54.780   0.010  64.877  1.00 31.04      B
ATOM   4412  CD2 TRP B 717      54.454  -0.438  66.203  1.00 29.45      B
ATOM   4413  CE2 TRP B 717      53.559  -1.521  66.071  1.00 29.85      B
ATOM   4414  CE3 TRP B 717      54.828  -0.029  67.483  1.00 30.32      B
ATOM   4415  CD1 TRP B 717      54.091  -0.807  64.024  1.00 30.88      B
ATOM   4416  NE1 TRP B 717      53.353  -1.724  64.736  1.00 29.32      B
ATOM   4417  CZ2 TRP B 717      53.027  -2.199  67.172  1.00 33.01      B
ATOM   4418  CZ3 TRP B 717      54.295  -0.706  68.583  1.00 33.00      B
ATOM   4419  CH2 TRP B 717      53.406  -1.778  68.416  1.00 32.26      B
ATOM   4420  C   TRP B 717      56.207   3.611  64.925  1.00 25.13      B
ATOM   4421  O   TRP B 717      56.995   3.961  65.782  1.00 27.18      B
ATOM   4422  N   SER B 718      56.163   4.189  63.743  1.00 24.84      B
ATOM   4423  CA  SER B 718      57.127   5.212  63.423  1.00 24.34      B
ATOM   4424  CB  SER B 718      58.314   4.536  62.727  1.00 24.77      B
ATOM   4425  OG  SER B 718      59.315   5.464  62.352  1.00 29.36      B
```

```
ATOM   4426  C   SER B 718      56.477   6.265  62.533  1.00 23.95      B
ATOM   4427  O   SER B 718      55.668   5.949  61.663  1.00 24.34      B
ATOM   4428  N   VAL B 719      56.813   7.521  62.754  1.00 21.34      B
ATOM   4429  CA  VAL B 719      56.236   8.549  61.934  1.00 20.74      B
ATOM   4430  CB  VAL B 719      55.041   9.202  62.663  1.00 20.34      B
ATOM   4431  CG1 VAL B 719      55.531  10.069  63.799  1.00 20.79      B
ATOM   4432  CG2 VAL B 719      54.182   9.964  61.685  1.00 20.98      B
ATOM   4433  C   VAL B 719      57.355   9.538  61.608  1.00 21.48      B
ATOM   4434  O   VAL B 719      58.204   9.840  62.452  1.00 21.37      B
ATOM   4435  N   ASN B 720      57.391  10.001  60.368  1.00 20.75      B
ATOM   4436  CA  ASN B 720      58.434  10.915  59.950  1.00 20.33      B
ATOM   4437  CB  ASN B 720      59.582  10.130  59.331  1.00 19.95      B
ATOM   4438  CG  ASN B 720      60.744  11.013  58.939  1.00 20.71      B
ATOM   4439  OD1 ASN B 720      60.570  12.186  58.613  1.00 22.75      B
ATOM   4440  ND2 ASN B 720      61.934  10.452  58.960  1.00 19.81      B
ATOM   4441  C   ASN B 720      57.831  11.792  58.885  1.00 21.17      B
ATOM   4442  O   ASN B 720      57.037  11.318  58.078  1.00 23.00      B
ATOM   4443  N   PHE B 721      58.187  13.067  58.850  1.00 20.66      B
ATOM   4444  CA  PHE B 721      57.630  13.907  57.791  1.00 21.75      B
ATOM   4445  CB  PHE B 721      56.339  14.591  58.289  1.00 17.46      B
ATOM   4446  CG  PHE B 721      56.556  15.653  59.312  1.00 14.32      B
ATOM   4447  CD1 PHE B 721      56.870  16.939  58.921  1.00 10.85      B
ATOM   4448  CD2 PHE B 721      56.404  15.387  60.660  1.00 11.84      B
ATOM   4449  CE1 PHE B 721      57.028  17.953  59.855  1.00 10.06      B
ATOM   4450  CE2 PHE B 721      56.561  16.405  61.607  1.00 13.14      B
ATOM   4451  CZ  PHE B 721      56.873  17.693  61.198  1.00 12.02      B
ATOM   4452  C   PHE B 721      58.656  14.902  57.259  1.00 22.48      B
ATOM   4453  O   PHE B 721      59.528  15.344  58.000  1.00 21.67      B
ATOM   4454  N   LYS B 722      58.584  15.205  55.961  1.00 24.01      B
ATOM   4455  CA  LYS B 722      59.508  16.161  55.320  1.00 24.93      B
ATOM   4456  CB  LYS B 722      60.752  15.450  54.783  1.00 25.59      B
ATOM   4457  CG  LYS B 722      61.838  15.134  55.800  1.00 27.22      B
ATOM   4458  CD  LYS B 722      62.834  16.283  55.958  0.00 27.08      B
ATOM   4459  CE  LYS B 722      62.210  17.519  56.576  0.00 27.46      B
ATOM   4460  NZ  LYS B 722      63.225  18.601  56.697  0.00 27.62      B
ATOM   4461  C   LYS B 722      58.838  16.863  54.151  1.00 24.47      B
ATOM   4462  O   LYS B 722      58.571  16.242  53.121  1.00 25.21      B
ATOM   4463  N   GLY B 723      58.569  18.153  54.298  1.00 24.23      B
ATOM   4464  CA  GLY B 723      57.937  18.872  53.209  1.00 26.31      B
ATOM   4465  C   GLY B 723      56.464  18.536  53.019  1.00 28.74      B
ATOM   4466  O   GLY B 723      55.694  18.529  53.979  1.00 29.75      B
ATOM   4467  N   LYS B 724      56.057  18.235  51.794  1.00 28.84      B
ATOM   4468  CA  LYS B 724      54.652  17.941  51.530  1.00 29.80      B
ATOM   4469  CB  LYS B 724      54.352  18.219  50.074  1.00 31.52      B
ATOM   4470  CG  LYS B 724      55.436  17.698  49.171  1.00 32.34      B
ATOM   4471  CD  LYS B 724      54.881  16.783  48.115  1.00 33.78      B
ATOM   4472  CE  LYS B 724      55.974  16.447  47.107  1.00 35.08      B
ATOM   4473  NZ  LYS B 724      56.379  17.659  46.344  1.00 33.47      B
ATOM   4474  C   LYS B 724      54.184  16.535  51.841  1.00 29.68      B
ATOM   4475  O   LYS B 724      52.988  16.260  51.801  1.00 28.58      B
ATOM   4476  N   THR B 725      55.121  15.643  52.135  1.00 29.01      B
ATOM   4477  CA  THR B 725      54.768  14.261  52.412  1.00 28.07      B
ATOM   4478  CB  THR B 725      55.459  13.315  51.372  1.00 28.24      B
ATOM   4479  OG1 THR B 725      55.740  12.040  51.957  1.00 28.44      B
```

```
ATOM   4480  CG2 THR B 725      56.732  13.943  50.850  1.00 29.05      B
ATOM   4481  C   THR B 725      55.081  13.853  53.847  1.00 27.60      B
ATOM   4482  O   THR B 725      56.070  14.292  54.445  1.00 27.85      B
ATOM   4483  N   LEU B 726      54.190  13.036  54.399  1.00 26.00      B
ATOM   4484  CA  LEU B 726      54.310  12.528  55.755  1.00 24.86      B
ATOM   4485  CB  LEU B 726      53.147  13.030  56.612  1.00 23.41      B
ATOM   4486  CG  LEU B 726      52.907  12.266  57.924  1.00 21.65      B
ATOM   4487  CD1 LEU B 726      54.123  12.369  58.805  1.00 24.41      B
ATOM   4488  CD2 LEU B 726      51.698  12.816  58.643  1.00 21.21      B
ATOM   4489  C   LEU B 726      54.254  11.014  55.677  1.00 25.90      B
ATOM   4490  O   LEU B 726      53.370  10.464  55.019  1.00 27.58      B
ATOM   4491  N   VAL B 727      55.196  10.329  56.315  1.00 24.78      B
ATOM   4492  CA  VAL B 727      55.151   8.875  56.283  1.00 25.06      B
ATOM   4493  CB  VAL B 727      56.388   8.256  55.556  1.00 23.86      B
ATOM   4494  CG1 VAL B 727      56.432   8.730  54.129  1.00 22.56      B
ATOM   4495  CG2 VAL B 727      57.678   8.571  56.296  1.00 23.51      B
ATOM   4496  C   VAL B 727      55.009   8.257  57.680  1.00 25.61      B
ATOM   4497  O   VAL B 727      55.637   8.717  58.641  1.00 25.40      B
ATOM   4498  N   ALA B 728      54.163   7.224  57.775  1.00 26.51      B
ATOM   4499  CA  ALA B 728      53.898   6.501  59.028  1.00 27.01      B
ATOM   4500  CB  ALA B 728      52.656   7.087  59.692  1.00 25.86      B
ATOM   4501  C   ALA B 728      53.734   4.960  58.886  1.00 27.72      B
ATOM   4502  O   ALA B 728      52.981   4.480  58.039  1.00 28.25      B
ATOM   4503  N   ALA B 729      54.457   4.204  59.718  1.00 29.53      B
ATOM   4504  CA  ALA B 729      54.401   2.735  59.745  1.00 30.38      B
ATOM   4505  CB  ALA B 729      55.761   2.150  60.042  1.00 26.88      B
ATOM   4506  C   ALA B 729      53.441   2.404  60.876  1.00 32.48      B
ATOM   4507  O   ALA B 729      53.692   2.754  62.036  1.00 32.95      B
ATOM   4508  N   VAL B 730      52.358   1.710  60.541  1.00 34.76      B
ATOM   4509  CA  VAL B 730      51.326   1.409  61.520  1.00 36.48      B
ATOM   4510  CB  VAL B 730      50.133   2.339  61.277  1.00 35.80      B
ATOM   4511  CG1 VAL B 730      50.546   3.802  61.484  1.00 35.67      B
ATOM   4512  CG2 VAL B 730      49.642   2.148  59.859  1.00 35.12      B
ATOM   4513  C   VAL B 730      50.819  -0.022  61.471  1.00 37.73      B
ATOM   4514  O   VAL B 730      51.069  -0.738  60.507  1.00 39.94      B
ATOM   4515  N   GLU B 731      50.102  -0.422  62.520  1.00 38.43      B
ATOM   4516  CA  GLU B 731      49.509  -1.755  62.608  1.00 38.21      B
ATOM   4517  CB  GLU B 731      49.851  -2.413  63.929  1.00 37.52      B
ATOM   4518  CG  GLU B 731      49.515  -3.869  63.933  1.00 39.46      B
ATOM   4519  CD  GLU B 731      49.255  -4.398  65.328  1.00 41.40      B
ATOM   4520  OE1 GLU B 731      48.163  -4.105  65.873  1.00 41.33      B
ATOM   4521  OE2 GLU B 731      50.140  -5.101  65.877  1.00 42.25      B
ATOM   4522  C   GLU B 731      47.996  -1.611  62.504  1.00 39.22      B
ATOM   4523  O   GLU B 731      47.393  -0.781  63.189  1.00 38.41      B
ATOM   4524  N   LYS B 732      47.382  -2.424  61.652  1.00 41.10      B
ATOM   4525  CA  LYS B 732      45.938  -2.358  61.449  1.00 43.00      B
ATOM   4526  CB  LYS B 732      45.635  -1.485  60.226  1.00 42.61      B
ATOM   4527  CG  LYS B 732      46.197  -0.077  60.333  0.00 43.37      B
ATOM   4528  CD  LYS B 732      46.607   0.492  58.981  0.00 43.64      B
ATOM   4529  CE  LYS B 732      45.431   0.678  58.036  0.00 43.89      B
ATOM   4530  NZ  LYS B 732      45.868   1.358  56.783  0.00 44.01      B
ATOM   4531  C   LYS B 732      45.381  -3.753  61.237  1.00 44.67      B
ATOM   4532  O   LYS B 732      45.879  -4.500  60.393  1.00 45.72      B
ATOM   4533  N   ASP B 733      44.350  -4.100  62.004  1.00 46.86      B
```

```
ATOM   4534  CA  ASP B 733      43.717  -5.417  61.898  1.00 48.20      B
ATOM   4535  CB  ASP B 733      43.098  -5.602  60.502  1.00 51.83      B
ATOM   4536  CG  ASP B 733      42.192  -6.824  60.411  1.00 54.62      B
ATOM   4537  OD1 ASP B 733      42.658  -7.894  59.947  1.00 55.49      B
ATOM   4538  OD2 ASP B 733      41.009  -6.708  60.812  1.00 55.81      B
ATOM   4539  C   ASP B 733      44.744  -6.520  62.159  1.00 46.65      B
ATOM   4540  O   ASP B 733      44.653  -7.621  61.614  1.00 46.27      B
ATOM   4541  N   GLY B 734      45.739  -6.203  62.977  1.00 45.55      B
ATOM   4542  CA  GLY B 734      46.749  -7.182  63.308  1.00 45.42      B
ATOM   4543  C   GLY B 734      47.792  -7.446  62.245  1.00 45.85      B
ATOM   4544  O   GLY B 734      48.334  -8.548  62.183  1.00 46.44      B
ATOM   4545  N   GLN B 735      48.073  -6.454  61.401  1.00 46.81      B
ATOM   4546  CA  GLN B 735      49.093  -6.599  60.355  1.00 47.05      B
ATOM   4547  CB  GLN B 735      48.461  -7.018  59.028  1.00 48.17      B
ATOM   4548  CG  GLN B 735      48.028  -8.461  59.027  1.00 52.88      B
ATOM   4549  CD  GLN B 735      46.961  -8.755  57.990  1.00 56.44      B
ATOM   4550  OE1 GLN B 735      46.245  -9.766  58.087  1.00 58.95      B
ATOM   4551  NE2 GLN B 735      46.840  -7.878  56.993  1.00 55.74      B
ATOM   4552  C   GLN B 735      49.897  -5.317  60.176  1.00 45.22      B
ATOM   4553  O   GLN B 735      49.597  -4.297  60.789  1.00 46.16      B
ATOM   4554  N   SER B 736      50.924  -5.394  59.336  1.00 42.48      B
ATOM   4555  CA  SER B 736      51.817  -4.278  59.061  1.00 39.38      B
ATOM   4556  CB  SER B 736      53.256  -4.791  59.003  1.00 40.16      B
ATOM   4557  OG  SER B 736      54.176  -3.797  59.394  1.00 40.72      B
ATOM   4558  C   SER B 736      51.468  -3.563  57.753  1.00 37.61      B
ATOM   4559  O   SER B 736      51.155  -4.193  56.734  1.00 37.66      B
ATOM   4560  N   PHE B 737      51.549  -2.239  57.797  1.00 33.84      B
ATOM   4561  CA  PHE B 737      51.228  -1.405  56.655  1.00 31.74      B
ATOM   4562  CB  PHE B 737      49.753  -1.006  56.716  1.00 32.02      B
ATOM   4563  CG  PHE B 737      48.802  -2.099  56.337  1.00 33.36      B
ATOM   4564  CD1 PHE B 737      48.776  -2.582  55.041  1.00 34.70      B
ATOM   4565  CD2 PHE B 737      47.894  -2.606  57.255  1.00 35.15      B
ATOM   4566  CE1 PHE B 737      47.857  -3.545  54.655  1.00 36.59      B
ATOM   4567  CE2 PHE B 737      46.964  -3.573  56.878  1.00 35.49      B
ATOM   4568  CZ  PHE B 737      46.946  -4.044  55.573  1.00 36.38      B
ATOM   4569  C   PHE B 737      52.077  -0.134  56.644  1.00 30.68      B
ATOM   4570  O   PHE B 737      52.650   0.254  57.665  1.00 31.62      B
ATOM   4571  N   LEU B 738      52.165   0.510  55.485  1.00 27.59      B
ATOM   4572  CA  LEU B 738      52.905   1.758  55.373  1.00 25.56      B
ATOM   4573  CB  LEU B 738      54.042   1.679  54.355  1.00 25.25      B
ATOM   4574  CG  LEU B 738      54.884   2.973  54.305  1.00 25.05      B
ATOM   4575  CD1 LEU B 738      55.668   3.104  55.614  1.00 22.91      B
ATOM   4576  CD2 LEU B 738      55.839   2.973  53.131  1.00 21.80      B
ATOM   4577  C   LEU B 738      51.947   2.841  54.922  1.00 24.87      B
ATOM   4578  O   LEU B 738      51.336   2.743  53.864  1.00 23.89      B
ATOM   4579  N   GLU B 739      51.820   3.882  55.728  1.00 24.71      B
ATOM   4580  CA  GLU B 739      50.940   4.976  55.372  1.00 23.29      B
ATOM   4581  CB  GLU B 739      50.206   5.458  56.612  1.00 24.09      B
ATOM   4582  CG  GLU B 739      48.692   5.452  56.495  1.00 28.17      B
ATOM   4583  CD  GLU B 739      48.058   4.066  56.517  1.00 28.62      B
ATOM   4584  OE1 GLU B 739      48.352   3.273  57.426  1.00 31.20      B
ATOM   4585  OE2 GLU B 739      47.232   3.782  55.633  1.00 28.53      B
ATOM   4586  C   GLU B 739      51.795   6.094  54.780  1.00 20.71      B
ATOM   4587  O   GLU B 739      52.906   6.329  55.235  1.00 20.52      B
```

```
ATOM   4588  N   ILE B 740      51.290   6.740  53.732  1.00 19.91      B
ATOM   4589  CA  ILE B 740      51.968   7.868  53.075  1.00 19.31      B
ATOM   4590  CB  ILE B 740      52.572   7.473  51.720  1.00 17.66      B
ATOM   4591  CG2 ILE B 740      53.171   8.701  51.030  1.00 15.65      B
ATOM   4592  CG1 ILE B 740      53.604   6.379  51.926  1.00 16.52      B
ATOM   4593  CD1 ILE B 740      54.155   5.833  50.629  1.00 18.73      B
ATOM   4594  C   ILE B 740      50.891   8.923  52.849  1.00 19.07      B
ATOM   4595  O   ILE B 740      49.886   8.655  52.209  1.00 19.78      B
ATOM   4596  N   LEU B 741      51.106  10.111  53.395  1.00 19.72      B
ATOM   4597  CA  LEU B 741      50.151  11.188  53.259  1.00 21.30      B
ATOM   4598  CB  LEU B 741      49.728  11.648  54.645  1.00 22.07      B
ATOM   4599  CG  LEU B 741      49.077  10.572  55.530  1.00 23.25      B
ATOM   4600  CD1 LEU B 741      48.660  11.188  56.855  1.00 23.41      B
ATOM   4601  CD2 LEU B 741      47.856   9.989  54.825  1.00 23.48      B
ATOM   4602  C   LEU B 741      50.732  12.357  52.461  1.00 22.75      B
ATOM   4603  O   LEU B 741      51.891  12.745  52.656  1.00 24.38      B
ATOM   4604  N   ASP B 742      49.918  12.918  51.571  1.00 23.48      B
ATOM   4605  CA  ASP B 742      50.324  14.032  50.711  1.00 24.55      B
ATOM   4606  CB  ASP B 742      49.931  13.723  49.276  1.00 26.67      B
ATOM   4607  CG  ASP B 742      50.733  14.515  48.271  1.00 28.63      B
ATOM   4608  OD1 ASP B 742      50.840  15.760  48.424  1.00 28.82      B
ATOM   4609  OD2 ASP B 742      51.245  13.879  47.328  1.00 28.63      B
ATOM   4610  C   ASP B 742      49.688  15.363  51.103  1.00 25.06      B
ATOM   4611  O   ASP B 742      48.481  15.436  51.305  1.00 26.84      B
ATOM   4612  N   PHE B 743      50.484  16.423  51.183  1.00 25.71      B
ATOM   4613  CA  PHE B 743      49.943  17.731  51.558  1.00 27.52      B
ATOM   4614  CB  PHE B 743      50.486  18.191  52.912  1.00 26.16      B
ATOM   4615  CG  PHE B 743      49.997  17.388  54.073  1.00 24.94      B
ATOM   4616  CD1 PHE B 743      50.565  16.158  54.378  1.00 24.17      B
ATOM   4617  CD2 PHE B 743      48.980  17.887  54.890  1.00 23.91      B
ATOM   4618  CE1 PHE B 743      50.132  15.437  55.490  1.00 24.90      B
ATOM   4619  CE2 PHE B 743      48.537  17.184  56.000  1.00 21.83      B
ATOM   4620  CZ  PHE B 743      49.111  15.957  56.306  1.00 23.09      B
ATOM   4621  C   PHE B 743      50.249  18.808  50.530  1.00 29.26      B
ATOM   4622  O   PHE B 743      50.140  20.005  50.808  1.00 29.97      B
ATOM   4623  N   SER B 744      50.646  18.372  49.344  1.00 30.92      B
ATOM   4624  CA  SER B 744      50.955  19.277  48.245  1.00 32.47      B
ATOM   4625  CB  SER B 744      51.761  18.531  47.188  1.00 32.25      B
ATOM   4626  OG  SER B 744      51.080  17.346  46.824  1.00 29.83      B
ATOM   4627  C   SER B 744      49.649  19.790  47.629  1.00 34.01      B
ATOM   4628  O   SER B 744      49.524  21.028  47.432  1.00 35.67      B
ATOM   4629  OXT SER B 744      48.778  18.934  47.348  1.00 33.32      B
ATOM   4630  CB  SER C   2      79.559  36.638  46.340  1.00 43.57      C
ATOM   4631  OG  SER C   2      79.993  37.690  45.505  1.00 44.36      C
ATOM   4632  C   SER C   2      78.062  35.376  44.763  1.00 44.40      C
ATOM   4633  O   SER C   2      78.864  34.452  44.588  1.00 45.41      C
ATOM   4634  N   SER C   2      77.555  35.428  47.144  1.00 45.64      C
ATOM   4635  CA  SER C   2      78.115  36.241  46.021  1.00 44.62      C
ATOM   4636  N   ASN C   3      77.108  35.678  43.890  1.00 43.20      C
ATOM   4637  CA  ASN C   3      76.921  34.908  42.666  1.00 41.97      C
ATOM   4638  CB  ASN C   3      75.435  34.551  42.505  1.00 43.04      C
ATOM   4639  CG  ASN C   3      74.952  33.552  43.535  1.00 43.55      C
ATOM   4640  OD1 ASN C   3      75.330  32.375  43.512  1.00 43.93      C
ATOM   4641  ND2 ASN C   3      74.105  34.017  44.448  1.00 43.67      C
```

```
ATOM   4642  C   ASN C   3      77.392  35.617  41.399  1.00 40.54      C
ATOM   4643  O   ASN C   3      77.723  36.800  41.401  1.00 40.39      C
ATOM   4644  N   VAL C   4      77.408  34.868  40.306  1.00 39.54      C
ATOM   4645  CA  VAL C   4      77.794  35.409  39.014  1.00 37.85      C
ATOM   4646  CB  VAL C   4      79.259  35.135  38.677  1.00 37.25      C
ATOM   4647  CG1 VAL C   4      80.128  36.252  39.212  1.00 37.46      C
ATOM   4648  CG2 VAL C   4      79.678  33.798  39.261  1.00 36.73      C
ATOM   4649  C   VAL C   4      76.959  34.717  37.975  1.00 36.19      C
ATOM   4650  O   VAL C   4      76.617  33.547  38.128  1.00 37.44      C
ATOM   4651  N   VAL C   5      76.627  35.440  36.917  1.00 33.92      C
ATOM   4652  CA  VAL C   5      75.844  34.864  35.846  1.00 31.07      C
ATOM   4653  CB  VAL C   5      74.812  35.871  35.315  1.00 29.79      C
ATOM   4654  CG1 VAL C   5      74.186  35.342  34.041  1.00 30.11      C
ATOM   4655  CG2 VAL C   5      73.735  36.100  36.359  1.00 28.61      C
ATOM   4656  C   VAL C   5      76.731  34.410  34.693  1.00 29.84      C
ATOM   4657  O   VAL C   5      77.601  35.147  34.233  1.00 29.90      C
ATOM   4658  N   LEU C   6      76.513  33.177  34.251  1.00 29.14      C
ATOM   4659  CA  LEU C   6      77.236  32.597  33.116  1.00 28.08      C
ATOM   4660  CB  LEU C   6      77.863  31.253  33.510  1.00 27.11      C
ATOM   4661  CG  LEU C   6      78.872  31.221  34.675  1.00 24.97      C
ATOM   4662  CD1 LEU C   6      79.528  29.845  34.700  1.00 24.15      C
ATOM   4663  CD2 LEU C   6      79.919  32.293  34.529  1.00 22.63      C
ATOM   4664  C   LEU C   6      76.201  32.405  31.990  1.00 27.51      C
ATOM   4665  O   LEU C   6      75.218  31.673  32.139  1.00 26.06      C
ATOM   4666  N   VAL C   7      76.422  33.083  30.869  1.00 28.04      C
ATOM   4667  CA  VAL C   7      75.498  33.035  29.732  1.00 29.08      C
ATOM   4668  CB  VAL C   7      75.410  34.425  29.046  1.00 30.10      C
ATOM   4669  CG1 VAL C   7      74.517  34.349  27.805  1.00 30.31      C
ATOM   4670  CG2 VAL C   7      74.887  35.454  30.033  1.00 28.75      C
ATOM   4671  C   VAL C   7      75.861  31.988  28.678  1.00 29.01      C
ATOM   4672  O   VAL C   7      77.008  31.913  28.226  1.00 28.23      C
ATOM   4673  N   SER C   8      74.865  31.191  28.291  1.00 28.51      C
ATOM   4674  CA  SER C   8      75.063  30.147  27.296  1.00 27.88      C
ATOM   4675  CB  SER C   8      74.009  29.037  27.418  1.00 28.20      C
ATOM   4676  OG  SER C   8      72.804  29.396  26.748  1.00 25.94      C
ATOM   4677  C   SER C   8      74.965  30.741  25.898  1.00 28.40      C
ATOM   4678  O   SER C   8      74.359  31.803  25.707  1.00 27.07      C
ATOM   4679  N   GLY C   9      75.574  30.034  24.941  1.00 27.46      C
ATOM   4680  CA  GLY C   9      75.569  30.450  23.553  1.00 26.64      C
ATOM   4681  C   GLY C   9      74.142  30.602  23.067  1.00 26.05      C
ATOM   4682  O   GLY C   9      73.874  31.296  22.085  1.00 26.15      C
ATOM   4683  N   GLU C  10      73.219  29.941  23.752  1.00 24.38      C
ATOM   4684  CA  GLU C  10      71.824  30.034  23.400  1.00 23.90      C
ATOM   4685  CB  GLU C  10      71.116  28.716  23.732  1.00 24.63      C
ATOM   4686  CG  GLU C  10      71.338  27.635  22.678  1.00 29.19      C
ATOM   4687  CD  GLU C  10      71.102  26.213  23.204  1.00 33.43      C
ATOM   4688  OE1 GLU C  10      70.758  25.307  22.400  1.00 35.21      C
ATOM   4689  OE2 GLU C  10      71.281  25.992  24.420  1.00 36.33      C
ATOM   4690  C   GLU C  10      71.186  31.221  24.133  1.00 23.12      C
ATOM   4691  O   GLU C  10      69.975  31.374  24.128  1.00 20.55      C
ATOM   4692  N   GLY C  11      72.008  32.064  24.756  1.00 25.05      C
ATOM   4693  CA  GLY C  11      71.491  33.228  25.458  1.00 26.75      C
ATOM   4694  C   GLY C  11      70.939  33.036  26.861  1.00 29.02      C
ATOM   4695  O   GLY C  11      70.676  34.022  27.557  1.00 28.98      C
```

ATOM	4696	N	GLU	C	12	70.757	31.782	27.276	1.00	29.73	C
ATOM	4697	CA	GLU	C	12	70.238	31.469	28.604	1.00	29.91	C
ATOM	4698	CB	GLU	C	12	69.778	30.009	28.657	1.00	29.67	C
ATOM	4699	CG	GLU	C	12	68.537	29.805	27.817	1.00	29.78	C
ATOM	4700	CD	GLU	C	12	67.792	28.516	28.112	1.00	31.45	C
ATOM	4701	OE1	GLU	C	12	68.320	27.419	27.801	1.00	31.80	C
ATOM	4702	OE2	GLU	C	12	66.663	28.603	28.651	1.00	32.30	C
ATOM	4703	C	GLU	C	12	71.231	31.769	29.730	1.00	31.37	C
ATOM	4704	O	GLU	C	12	72.364	31.288	29.723	1.00	31.63	C
ATOM	4705	N	ARG	C	13	70.793	32.579	30.693	1.00	32.45	C
ATOM	4706	CA	ARG	C	13	71.642	32.983	31.807	1.00	33.31	C
ATOM	4707	CB	ARG	C	13	71.215	34.341	32.335	1.00	33.47	C
ATOM	4708	CG	ARG	C	13	70.328	35.124	31.392	1.00	35.00	C
ATOM	4709	CD	ARG	C	13	69.909	36.383	32.092	1.00	35.56	C
ATOM	4710	NE	ARG	C	13	71.082	37.195	32.375	1.00	39.21	C
ATOM	4711	CZ	ARG	C	13	71.210	37.997	33.423	1.00	40.03	C
ATOM	4712	NH1	ARG	C	13	70.231	38.093	34.310	1.00	39.27	C
ATOM	4713	NH2	ARG	C	13	72.310	38.726	33.566	1.00	40.62	C
ATOM	4714	C	ARG	C	13	71.607	31.997	32.949	1.00	33.28	C
ATOM	4715	O	ARG	C	13	70.534	31.584	33.387	1.00	33.83	C
ATOM	4716	N	PHE	C	14	72.790	31.626	33.431	1.00	33.28	C
ATOM	4717	CA	PHE	C	14	72.916	30.692	34.545	1.00	32.01	C
ATOM	4718	CB	PHE	C	14	73.791	29.488	34.180	1.00	32.03	C
ATOM	4719	CG	PHE	C	14	73.173	28.552	33.175	1.00	32.79	C
ATOM	4720	CD1	PHE	C	14	73.005	28.935	31.850	1.00	33.70	C
ATOM	4721	CD2	PHE	C	14	72.815	27.256	33.545	1.00	32.47	C
ATOM	4722	CE1	PHE	C	14	72.491	28.032	30.910	1.00	34.61	C
ATOM	4723	CE2	PHE	C	14	72.301	26.349	32.620	1.00	30.80	C
ATOM	4724	CZ	PHE	C	14	72.141	26.731	31.300	1.00	31.82	C
ATOM	4725	C	PHE	C	14	73.560	31.394	35.733	1.00	31.30	C
ATOM	4726	O	PHE	C	14	74.669	31.918	35.633	1.00	30.38	C
ATOM	4727	N	THR	C	15	72.860	31.403	36.857	1.00	30.28	C
ATOM	4728	CA	THR	C	15	73.387	32.013	38.066	1.00	29.27	C
ATOM	4729	CB	THR	C	15	72.253	32.635	38.900	1.00	28.06	C
ATOM	4730	OG1	THR	C	15	71.567	33.612	38.111	1.00	27.43	C
ATOM	4731	CG2	THR	C	15	72.801	33.282	40.158	1.00	25.34	C
ATOM	4732	C	THR	C	15	74.060	30.925	38.901	1.00	29.98	C
ATOM	4733	O	THR	C	15	73.521	29.827	39.032	1.00	30.73	C
ATOM	4734	N	VAL	C	16	75.244	31.211	39.435	1.00	30.04	C
ATOM	4735	CA	VAL	C	16	75.943	30.254	40.291	1.00	31.88	C
ATOM	4736	CB	VAL	C	16	76.853	29.283	39.491	1.00	32.07	C
ATOM	4737	CG1	VAL	C	16	76.035	28.547	38.455	1.00	35.42	C
ATOM	4738	CG2	VAL	C	16	77.988	30.034	38.823	1.00	34.64	C
ATOM	4739	C	VAL	C	16	76.793	30.991	41.327	1.00	32.89	C
ATOM	4740	O	VAL	C	16	77.097	32.176	41.168	1.00	32.60	C
ATOM	4741	N	ASP	C	17	77.170	30.286	42.390	1.00	33.45	C
ATOM	4742	CA	ASP	C	17	77.976	30.874	43.455	1.00	33.69	C
ATOM	4743	CB	ASP	C	17	78.117	29.888	44.618	1.00	35.66	C
ATOM	4744	CG	ASP	C	17	79.027	30.419	45.727	1.00	38.16	C
ATOM	4745	OD1	ASP	C	17	78.721	31.520	46.269	1.00	38.20	C
ATOM	4746	OD2	ASP	C	17	80.037	29.741	46.047	1.00	36.91	C
ATOM	4747	C	ASP	C	17	79.347	31.221	42.911	1.00	33.45	C
ATOM	4748	O	ASP	C	17	80.034	30.352	42.391	1.00	32.08	C
ATOM	4749	N	LYS	C	18	79.768	32.475	43.045	1.00	35.48	C

```
ATOM   4750  CA  LYS C  18      81.068  32.853  42.495  1.00 39.15      C
ATOM   4751  CB  LYS C  18      81.378  34.325  42.766  1.00 40.50      C
ATOM   4752  CG  LYS C  18      81.886  34.630  44.144  1.00 45.70      C
ATOM   4753  CD  LYS C  18      82.169  36.128  44.285  1.00 48.13      C
ATOM   4754  CE  LYS C  18      83.245  36.589  43.318  1.00 48.38      C
ATOM   4755  NZ  LYS C  18      84.546  35.898  43.581  1.00 49.06      C
ATOM   4756  C   LYS C  18      82.212  31.978  42.993  1.00 38.99      C
ATOM   4757  O   LYS C  18      83.109  31.638  42.228  1.00 38.11      C
ATOM   4758  N   LYS C  19      82.177  31.596  44.263  1.00 39.59      C
ATOM   4759  CA  LYS C  19      83.232  30.759  44.813  1.00 38.98      C
ATOM   4760  CB  LYS C  19      82.940  30.429  46.274  0.00 39.52      C
ATOM   4761  CG  LYS C  19      84.077  29.703  46.968  0.00 40.25      C
ATOM   4762  CD  LYS C  19      83.738  29.363  48.404  0.00 40.84      C
ATOM   4763  CE  LYS C  19      82.586  28.380  48.468  0.00 41.18      C
ATOM   4764  NZ  LYS C  19      82.206  28.077  49.871  0.00 41.44      C
ATOM   4765  C   LYS C  19      83.364  29.470  44.010  1.00 38.49      C
ATOM   4766  O   LYS C  19      84.475  29.025  43.725  1.00 37.49      C
ATOM   4767  N   ILE C  20      82.223  28.877  43.651  1.00 39.86      C
ATOM   4768  CA  ILE C  20      82.167  27.631  42.858  1.00 40.16      C
ATOM   4769  CB  ILE C  20      80.725  27.037  42.836  1.00 39.38      C
ATOM   4770  CG2 ILE C  20      80.705  25.698  42.109  1.00 38.50      C
ATOM   4771  CG1 ILE C  20      80.225  26.858  44.270  1.00 39.70      C
ATOM   4772  CD1 ILE C  20      78.801  26.351  44.371  1.00 41.15      C
ATOM   4773  C   ILE C  20      82.588  27.949  41.421  1.00 40.51      C
ATOM   4774  O   ILE C  20      83.424  27.272  40.841  1.00 39.84      C
ATOM   4775  N   ALA C  21      81.999  28.999  40.865  1.00 41.64      C
ATOM   4776  CA  ALA C  21      82.312  29.423  39.524  1.00 43.06      C
ATOM   4777  CB  ALA C  21      81.635  30.753  39.229  1.00 43.43      C
ATOM   4778  C   ALA C  21      83.818  29.554  39.349  1.00 43.95      C
ATOM   4779  O   ALA C  21      84.353  29.186  38.307  1.00 45.27      C
ATOM   4780  N   GLU C  22      84.506  30.090  40.354  1.00 44.60      C
ATOM   4781  CA  GLU C  22      85.958  30.254  40.266  1.00 44.95      C
ATOM   4782  CB  GLU C  22      86.546  30.773  41.582  1.00 47.05      C
ATOM   4783  CG  GLU C  22      86.200  32.217  41.915  1.00 50.65      C
ATOM   4784  CD  GLU C  22      87.063  32.769  43.035  1.00 52.85      C
ATOM   4785  OE1 GLU C  22      87.098  32.164  44.125  1.00 54.88      C
ATOM   4786  OE2 GLU C  22      87.716  33.809  42.826  1.00 54.85      C
ATOM   4787  C   GLU C  22      86.652  28.949  39.898  1.00 43.86      C
ATOM   4788  O   GLU C  22      87.851  28.933  39.637  1.00 43.78      C
ATOM   4789  N   ARG C  23      85.912  27.849  39.893  1.00 42.42      C
ATOM   4790  CA  ARG C  23      86.498  26.576  39.517  1.00 42.71      C
ATOM   4791  CB  ARG C  23      85.442  25.496  39.602  1.00 43.00      C
ATOM   4792  CG  ARG C  23      85.870  24.197  39.043  1.00 44.32      C
ATOM   4793  CD  ARG C  23      86.100  23.258  40.161  1.00 46.65      C
ATOM   4794  NE  ARG C  23      87.502  23.204  40.508  1.00 47.94      C
ATOM   4795  CZ  ARG C  23      87.967  22.532  41.548  1.00 48.45      C
ATOM   4796  NH1 ARG C  23      87.122  21.875  42.338  1.00 46.40      C
ATOM   4797  NH2 ARG C  23      89.274  22.493  41.768  1.00 50.58      C
ATOM   4798  C   ARG C  23      86.956  26.742  38.072  1.00 42.33      C
ATOM   4799  O   ARG C  23      87.703  25.926  37.536  1.00 41.75      C
ATOM   4800  N   SER C  24      86.461  27.812  37.458  1.00 42.76      C
ATOM   4801  CA  SER C  24      86.773  28.177  36.087  1.00 43.35      C
ATOM   4802  CB  SER C  24      85.531  28.757  35.406  1.00 42.29      C
ATOM   4803  OG  SER C  24      85.845  29.241  34.116  1.00 39.65      C
```

```
ATOM   4804  C   SER C  24      87.868  29.235  36.113  1.00 44.08      C
ATOM   4805  O   SER C  24      87.591  30.403  36.361  1.00 44.37      C
ATOM   4806  N   LEU C  25      89.109  28.830  35.875  1.00 45.48      C
ATOM   4807  CA  LEU C  25      90.217  29.773  35.875  1.00 47.35      C
ATOM   4808  CB  LEU C  25      91.490  29.117  35.350  1.00 48.27      C
ATOM   4809  CG  LEU C  25      92.107  28.027  36.219  1.00 48.77      C
ATOM   4810  CD1 LEU C  25      93.392  27.506  35.595  0.00 48.78      C
ATOM   4811  CD2 LEU C  25      92.365  28.610  37.598  1.00 48.53      C
ATOM   4812  C   LEU C  25      89.871  30.932  34.979  1.00 48.70      C
ATOM   4813  O   LEU C  25      90.293  32.064  35.233  1.00 48.05      C
ATOM   4814  N   LEU C  26      89.116  30.635  33.919  1.00 50.30      C
ATOM   4815  CA  LEU C  26      88.703  31.658  32.956  1.00 50.59      C
ATOM   4816  CB  LEU C  26      87.901  31.046  31.787  1.00 50.13      C
ATOM   4817  CG  LEU C  26      87.543  31.994  30.621  1.00 49.31      C
ATOM   4818  CD1 LEU C  26      88.810  32.356  29.880  1.00 49.37      C
ATOM   4819  CD2 LEU C  26      86.542  31.346  29.655  1.00 49.24      C
ATOM   4820  C   LEU C  26      87.857  32.687  33.689  1.00 50.59      C
ATOM   4821  O   LEU C  26      88.005  33.888  33.478  1.00 50.43      C
ATOM   4822  N   LEU C  27      86.980  32.210  34.562  1.00 51.20      C
ATOM   4823  CA  LEU C  27      86.132  33.103  35.325  1.00 53.37      C
ATOM   4824  CB  LEU C  27      84.930  32.324  35.871  1.00 54.39      C
ATOM   4825  CG  LEU C  27      83.811  33.095  36.583  1.00 55.55      C
ATOM   4826  CD1 LEU C  27      84.258  33.408  37.990  1.00 56.54      C
ATOM   4827  CD2 LEU C  27      83.445  34.376  35.817  1.00 55.58      C
ATOM   4828  C   LEU C  27      86.947  33.775  36.446  1.00 54.11      C
ATOM   4829  O   LEU C  27      86.669  34.918  36.822  1.00 54.13      C
ATOM   4830  N   LYS C  28      87.960  33.077  36.961  1.00 54.29      C
ATOM   4831  CA  LYS C  28      88.816  33.650  37.993  1.00 54.46      C
ATOM   4832  CB  LYS C  28      89.825  32.623  38.506  1.00 54.18      C
ATOM   4833  CG  LYS C  28      89.252  31.586  39.446  1.00 54.09      C
ATOM   4834  CD  LYS C  28      90.359  30.727  40.048  0.00 54.84      C
ATOM   4835  CE  LYS C  28      91.404  31.584  40.756  0.00 55.16      C
ATOM   4836  NZ  LYS C  28      90.817  32.412  41.846  0.00 55.54      C
ATOM   4837  C   LYS C  28      89.565  34.851  37.408  1.00 55.03      C
ATOM   4838  O   LYS C  28      89.502  35.943  37.956  1.00 54.89      C
ATOM   4839  N   ASN C  29      90.269  34.657  36.295  1.00 56.14      C
ATOM   4840  CA  ASN C  29      91.006  35.758  35.671  1.00 57.16      C
ATOM   4841  CB  ASN C  29      91.659  35.319  34.354  1.00 57.83      C
ATOM   4842  CG  ASN C  29      92.642  34.173  34.532  1.00 58.99      C
ATOM   4843  OD1 ASN C  29      93.170  33.633  33.558  1.00 59.61      C
ATOM   4844  ND2 ASN C  29      92.895  33.800  35.776  1.00 59.68      C
ATOM   4845  C   ASN C  29      90.071  36.923  35.375  1.00 57.45      C
ATOM   4846  O   ASN C  29      90.455  38.079  35.525  1.00 57.22      C
ATOM   4847  N   TYR C  30      88.849  36.620  34.943  1.00 57.89      C
ATOM   4848  CA  TYR C  30      87.882  37.664  34.615  1.00 58.66      C
ATOM   4849  CB  TYR C  30      86.516  37.039  34.317  1.00 57.87      C
ATOM   4850  CG  TYR C  30      85.636  37.872  33.409  1.00 56.71      C
ATOM   4851  CD1 TYR C  30      86.054  38.229  32.133  1.00 55.67      C
ATOM   4852  CE1 TYR C  30      85.231  38.968  31.282  1.00 55.50      C
ATOM   4853  CD2 TYR C  30      84.373  38.276  33.818  1.00 56.61      C
ATOM   4854  CE2 TYR C  30      83.539  39.014  32.979  1.00 56.59      C
ATOM   4855  CZ  TYR C  30      83.972  39.355  31.712  1.00 56.92      C
ATOM   4856  OH  TYR C  30      83.132  40.065  30.873  1.00 57.63      C
ATOM   4857  C   TYR C  30      87.787  38.649  35.783  1.00 60.59      C
```

```
ATOM   4858  O   TYR C  30      87.482  39.830  35.590  1.00 59.71      C
ATOM   4859  N   LEU C  31      88.062  38.146  36.989  1.00 62.33      C
ATOM   4860  CA  LEU C  31      88.047  38.932  38.230  1.00 62.29      C
ATOM   4861  CB  LEU C  31      89.371  39.712  38.370  1.00 62.08      C
ATOM   4862  CG  LEU C  31      89.853  40.603  37.215  1.00 61.04      C
ATOM   4863  CD1 LEU C  31      89.303  42.000  37.370  1.00 60.84      C
ATOM   4864  CD2 LEU C  31      91.363  40.639  37.205  1.00 61.22      C
ATOM   4865  C   LEU C  31      86.860  39.875  38.358  1.00 62.55      C
ATOM   4866  O   LEU C  31      85.754  39.555  37.917  1.00 63.88      C
ATOM   4867  N   ILE C  45      80.545  40.215  37.240  1.00 45.54      C
ATOM   4868  CA  ILE C  45      79.354  39.523  37.719  1.00 45.75      C
ATOM   4869  CB  ILE C  45      78.323  40.511  38.318  1.00 46.06      C
ATOM   4870  CG2 ILE C  45      77.704  41.376  37.213  1.00 43.89      C
ATOM   4871  CG1 ILE C  45      77.248  39.723  39.075  1.00 46.70      C
ATOM   4872  CD1 ILE C  45      76.128  40.574  39.614  1.00 48.94      C
ATOM   4873  C   ILE C  45      78.665  38.702  36.617  1.00 45.24      C
ATOM   4874  O   ILE C  45      78.069  37.659  36.904  1.00 45.32      C
ATOM   4875  N   VAL C  46      78.758  39.158  35.364  1.00 43.40      C
ATOM   4876  CA  VAL C  46      78.154  38.438  34.237  1.00 41.39      C
ATOM   4877  CB  VAL C  46      76.974  39.226  33.613  1.00 41.64      C
ATOM   4878  CG1 VAL C  46      76.308  38.378  32.531  1.00 41.02      C
ATOM   4879  CG2 VAL C  46      75.962  39.604  34.690  1.00 41.38      C
ATOM   4880  C   VAL C  46      79.154  38.131  33.123  1.00 39.66      C
ATOM   4881  O   VAL C  46      79.480  39.005  32.318  1.00 40.66      C
ATOM   4882  N   MSE C  47      79.635  36.892  33.071  1.00 38.75      C
ATOM   4883  CA  MSE C  47      80.597  36.501  32.039  1.00 37.26      C
ATOM   4884  CB  MSE C  47      81.753  35.691  32.641  1.00 38.19      C
ATOM   4885  CG  MSE C  47      82.901  35.488  31.668  1.00 40.50      C
ATOM   4886  SE  MSE C  47      84.215  34.179  32.219  1.00 47.69      C
ATOM   4887  CE  MSE C  47      83.332  32.527  31.723  1.00 41.93      C
ATOM   4888  C   MSE C  47      79.924  35.669  30.954  1.00 34.30      C
ATOM   4889  O   MSE C  47      79.108  34.793  31.246  1.00 32.32      C
ATOM   4890  N   PRO C  48      80.240  35.954  29.682  1.00 32.53      C
ATOM   4891  CD  PRO C  48      80.789  37.227  29.204  1.00 31.72      C
ATOM   4892  CA  PRO C  48      79.655  35.207  28.566  1.00 32.32      C
ATOM   4893  CB  PRO C  48      79.787  36.176  27.389  1.00 31.12      C
ATOM   4894  CG  PRO C  48      79.872  37.514  28.049  1.00 31.73      C
ATOM   4895  C   PRO C  48      80.408  33.895  28.302  1.00 31.55      C
ATOM   4896  O   PRO C  48      81.615  33.809  28.506  1.00 32.35      C
ATOM   4897  N   VAL C  49      79.696  32.864  27.874  1.00 30.22      C
ATOM   4898  CA  VAL C  49      80.347  31.609  27.553  1.00 29.45      C
ATOM   4899  CB  VAL C  49      79.832  30.440  28.418  1.00 30.65      C
ATOM   4900  CG1 VAL C  49      80.731  29.222  28.234  1.00 29.09      C
ATOM   4901  CG2 VAL C  49      79.803  30.851  29.872  1.00 31.28      C
ATOM   4902  C   VAL C  49      79.958  31.389  26.105  1.00 28.38      C
ATOM   4903  O   VAL C  49      79.011  30.660  25.798  1.00 28.07      C
ATOM   4904  N   PRO C  50      80.673  32.049  25.191  1.00 27.28      C
ATOM   4905  CD  PRO C  50      81.736  33.036  25.433  1.00 27.20      C
ATOM   4906  CA  PRO C  50      80.410  31.937  23.765  1.00 26.24      C
ATOM   4907  CB  PRO C  50      81.504  32.810  23.158  1.00 26.55      C
ATOM   4908  CG  PRO C  50      81.687  33.866  24.182  1.00 25.75      C
ATOM   4909  C   PRO C  50      80.426  30.516  23.202  1.00 26.07      C
ATOM   4910  O   PRO C  50      81.292  29.698  23.529  1.00 25.12      C
ATOM   4911  N   ASN C  51      79.447  30.247  22.347  1.00 25.23      C
```

```
ATOM   4912  CA  ASN C  51      79.317  28.975  21.668  1.00 25.26      C
ATOM   4913  CB  ASN C  51      80.446  28.820  20.660  1.00 26.35      C
ATOM   4914  CG  ASN C  51      80.554  30.005  19.737  1.00 27.98      C
ATOM   4915  OD1 ASN C  51      79.567  30.413  19.116  1.00 28.79      C
ATOM   4916  ND2 ASN C  51      81.752  30.578  19.644  1.00 27.02      C
ATOM   4917  C   ASN C  51      79.299  27.762  22.558  1.00 24.62      C
ATOM   4918  O   ASN C  51      80.090  26.861  22.374  1.00 25.28      C
ATOM   4919  N   VAL C  52      78.388  27.726  23.510  1.00 25.26      C
ATOM   4920  CA  VAL C  52      78.284  26.592  24.395  1.00 25.46      C
ATOM   4921  CB  VAL C  52      78.983  26.866  25.714  1.00 27.00      C
ATOM   4922  CG1 VAL C  52      78.759  25.698  26.668  1.00 26.64      C
ATOM   4923  CG2 VAL C  52      80.473  27.098  25.487  1.00 27.68      C
ATOM   4924  C   VAL C  52      76.808  26.404  24.685  1.00 27.92      C
ATOM   4925  O   VAL C  52      76.181  27.275  25.305  1.00 30.25      C
ATOM   4926  N   ARG C  53      76.246  25.278  24.249  1.00 28.81      C
ATOM   4927  CA  ARG C  53      74.824  25.012  24.478  1.00 29.52      C
ATOM   4928  CB  ARG C  53      74.393  23.688  23.845  1.00 32.39      C
ATOM   4929  CG  ARG C  53      74.401  23.661  22.337  1.00 37.27      C
ATOM   4930  CD  ARG C  53      73.908  22.307  21.839  1.00 42.50      C
ATOM   4931  NE  ARG C  53      74.746  21.181  22.276  1.00 47.26      C
ATOM   4932  CZ  ARG C  53      74.285  20.079  22.871  1.00 49.64      C
ATOM   4933  NH1 ARG C  53      72.984  19.945  23.114  1.00 48.76      C
ATOM   4934  NH2 ARG C  53      75.126  19.106  23.216  1.00 50.78      C
ATOM   4935  C   ARG C  53      74.465  24.959  25.964  1.00 28.83      C
ATOM   4936  O   ARG C  53      75.226  24.471  26.794  1.00 27.65      C
ATOM   4937  N   SER C  54      73.274  25.454  26.268  1.00 27.01      C
ATOM   4938  CA  SER C  54      72.769  25.467  27.613  1.00 24.06      C
ATOM   4939  CB  SER C  54      71.302  25.871  27.612  1.00 22.38      C
ATOM   4940  OG  SER C  54      71.159  27.162  27.056  1.00 20.31      C
ATOM   4941  C   SER C  54      72.946  24.093  28.246  1.00 24.61      C
ATOM   4942  O   SER C  54      73.676  23.948  29.223  1.00 26.72      C
ATOM   4943  N   SER C  55      72.306  23.071  27.698  1.00 23.42      C
ATOM   4944  CA  SER C  55      72.455  21.735  28.268  1.00 22.33      C
ATOM   4945  CB  SER C  55      71.922  20.684  27.304  1.00 19.49      C
ATOM   4946  OG  SER C  55      72.598  20.765  26.075  1.00 22.52      C
ATOM   4947  C   SER C  55      73.909  21.414  28.610  1.00 21.51      C
ATOM   4948  O   SER C  55      74.168  20.766  29.613  1.00 23.53      C
ATOM   4949  N   VAL C  56      74.851  21.884  27.795  1.00 20.84      C
ATOM   4950  CA  VAL C  56      76.274  21.624  28.031  1.00 20.83      C
ATOM   4951  CB  VAL C  56      77.137  21.998  26.757  1.00 20.76      C
ATOM   4952  CG1 VAL C  56      78.593  21.624  26.953  1.00 16.97      C
ATOM   4953  CG2 VAL C  56      76.583  21.284  25.514  1.00 20.88      C
ATOM   4954  C   VAL C  56      76.768  22.418  29.260  1.00 19.61      C
ATOM   4955  O   VAL C  56      77.375  21.849  30.172  1.00 18.87      C
ATOM   4956  N   LEU C  57      76.515  23.724  29.271  1.00 19.82      C
ATOM   4957  CA  LEU C  57      76.906  24.588  30.379  1.00 20.45      C
ATOM   4958  CB  LEU C  57      76.487  26.026  30.075  1.00 17.81      C
ATOM   4959  CG  LEU C  57      76.896  27.099  31.084  1.00 15.76      C
ATOM   4960  CD1 LEU C  57      78.375  27.066  31.281  1.00 14.13      C
ATOM   4961  CD2 LEU C  57      76.451  28.463  30.589  1.00 17.83      C
ATOM   4962  C   LEU C  57      76.231  24.116  31.678  1.00 21.81      C
ATOM   4963  O   LEU C  57      76.842  24.076  32.744  1.00 22.15      C
ATOM   4964  N   GLN C  58      74.956  23.777  31.588  1.00 22.64      C
ATOM   4965  CA  GLN C  58      74.255  23.311  32.757  1.00 24.92      C
```

```
ATOM   4966  CB  GLN C  58      72.811  22.991  32.418  1.00 25.24      C
ATOM   4967  CG  GLN C  58      72.079  22.366  33.567  1.00 27.25      C
ATOM   4968  CD  GLN C  58      70.636  22.144  33.271  1.00 28.40      C
ATOM   4969  OE1 GLN C  58      70.047  21.177  33.740  1.00 31.18      C
ATOM   4970  NE2 GLN C  58      70.043  23.041  32.500  1.00 29.28      C
ATOM   4971  C   GLN C  58      74.938  22.065  33.282  1.00 26.17      C
ATOM   4972  O   GLN C  58      75.060  21.872  34.487  1.00 27.72      C
ATOM   4973  N   LYS C  59      75.375  21.209  32.373  1.00 27.32      C
ATOM   4974  CA  LYS C  59      76.047  19.990  32.771  1.00 29.09      C
ATOM   4975  CB  LYS C  59      76.229  19.093  31.549  1.00 29.32      C
ATOM   4976  CG  LYS C  59      76.548  17.651  31.869  1.00 32.80      C
ATOM   4977  CD  LYS C  59      75.309  16.788  31.972  1.00 32.66      C
ATOM   4978  CE  LYS C  59      75.708  15.346  32.280  1.00 34.41      C
ATOM   4979  NZ  LYS C  59      74.566  14.374  32.116  1.00 36.74      C
ATOM   4980  C   LYS C  59      77.406  20.346  33.412  1.00 31.23      C
ATOM   4981  O   LYS C  59      77.793  19.750  34.418  1.00 32.05      C
ATOM   4982  N   VAL C  60      78.116  21.320  32.837  1.00 31.14      C
ATOM   4983  CA  VAL C  60      79.416  21.769  33.350  1.00 30.44      C
ATOM   4984  CB  VAL C  60      80.022  22.893  32.461  1.00 30.16      C
ATOM   4985  CG1 VAL C  60      81.236  23.514  33.139  1.00 28.33      C
ATOM   4986  CG2 VAL C  60      80.422  22.325  31.109  1.00 32.07      C
ATOM   4987  C   VAL C  60      79.310  22.314  34.767  1.00 31.68      C
ATOM   4988  O   VAL C  60      80.078  21.953  35.650  1.00 32.71      C
ATOM   4989  N   ILE C  61      78.356  23.204  34.969  1.00 32.12      C
ATOM   4990  CA  ILE C  61      78.140  23.804  36.262  1.00 31.24      C
ATOM   4991  CB  ILE C  61      77.021  24.824  36.170  1.00 31.54      C
ATOM   4992  CG2 ILE C  61      76.601  25.279  37.564  1.00 28.63      C
ATOM   4993  CG1 ILE C  61      77.497  25.982  35.297  1.00 31.49      C
ATOM   4994  CD1 ILE C  61      76.388  26.850  34.795  1.00 32.68      C
ATOM   4995  C   ILE C  61      77.780  22.749  37.289  1.00 31.52      C
ATOM   4996  O   ILE C  61      78.360  22.707  38.368  1.00 31.59      C
ATOM   4997  N   GLU C  62      76.836  21.881  36.955  1.00 31.93      C
ATOM   4998  CA  GLU C  62      76.443  20.861  37.907  1.00 33.23      C
ATOM   4999  CB  GLU C  62      75.295  20.025  37.375  1.00 32.43      C
ATOM   5000  CG  GLU C  62      75.721  18.813  36.636  1.00 34.09      C
ATOM   5001  CD  GLU C  62      74.649  17.762  36.649  1.00 35.90      C
ATOM   5002  OE1 GLU C  62      74.307  17.292  37.757  1.00 35.78      C
ATOM   5003  OE2 GLU C  62      74.143  17.408  35.558  1.00 37.89      C
ATOM   5004  C   GLU C  62      77.595  19.939  38.278  1.00 33.56      C
ATOM   5005  O   GLU C  62      77.462  19.096  39.161  1.00 34.70      C
ATOM   5006  N   TRP C  63      78.717  20.086  37.593  1.00 33.45      C
ATOM   5007  CA  TRP C  63      79.872  19.269  37.888  1.00 33.70      C
ATOM   5008  CB  TRP C  63      80.670  18.991  36.622  1.00 33.66      C
ATOM   5009  CG  TRP C  63      81.955  18.280  36.884  1.00 33.52      C
ATOM   5010  CD2 TRP C  63      83.211  18.876  37.231  1.00 32.28      C
ATOM   5011  CE2 TRP C  63      84.142  17.826  37.386  1.00 32.37      C
ATOM   5012  CE3 TRP C  63      83.639  20.196  37.429  1.00 31.95      C
ATOM   5013  CD1 TRP C  63      82.167  16.935  36.846  1.00 34.55      C
ATOM   5014  NE1 TRP C  63      83.481  16.653  37.143  1.00 34.74      C
ATOM   5015  CZ2 TRP C  63      85.476  18.049  37.726  1.00 32.07      C
ATOM   5016  CZ3 TRP C  63      84.965  20.424  37.768  1.00 31.44      C
ATOM   5017  CH2 TRP C  63      85.871  19.351  37.914  1.00 32.65      C
ATOM   5018  C   TRP C  63      80.726  20.067  38.853  1.00 34.67      C
ATOM   5019  O   TRP C  63      81.367  19.512  39.733  1.00 36.11      C
```

ATOM	5020	N	ALA	C	64	80.737	21.380	38.686	1.00	36.01	C
ATOM	5021	CA	ALA	C	64	81.537	22.234	39.551	1.00	38.09	C
ATOM	5022	CB	ALA	C	64	81.604	23.652	38.975	1.00	38.34	C
ATOM	5023	C	ALA	C	64	80.954	22.270	40.954	1.00	38.84	C
ATOM	5024	O	ALA	C	64	81.653	22.010	41.928	1.00	40.17	C
ATOM	5025	N	GLU	C	65	79.670	22.605	41.045	1.00	39.31	C
ATOM	5026	CA	GLU	C	65	78.981	22.675	42.322	1.00	39.42	C
ATOM	5027	CB	GLU	C	65	77.483	22.928	42.099	1.00	37.23	C
ATOM	5028	CG	GLU	C	65	77.202	24.210	41.330	1.00	34.34	C
ATOM	5029	CD	GLU	C	65	75.724	24.533	41.190	1.00	33.67	C
ATOM	5030	OE1	GLU	C	65	74.926	23.651	40.805	1.00	33.23	C
ATOM	5031	OE2	GLU	C	65	75.356	25.688	41.455	1.00	33.33	C
ATOM	5032	C	GLU	C	65	79.196	21.376	43.101	1.00	41.07	C
ATOM	5033	O	GLU	C	65	79.379	21.406	44.315	1.00	41.60	C
ATOM	5034	N	HIS	C	66	79.190	20.240	42.403	1.00	42.63	C
ATOM	5035	CA	HIS	C	66	79.391	18.944	43.059	1.00	44.78	C
ATOM	5036	CB	HIS	C	66	78.988	17.796	42.119	1.00	44.20	C
ATOM	5037	CG	HIS	C	66	79.334	16.420	42.622	1.00	44.62	C
ATOM	5038	CD2	HIS	C	66	78.548	15.363	42.937	1.00	43.92	C
ATOM	5039	ND1	HIS	C	66	80.634	15.972	42.740	1.00	45.83	C
ATOM	5040	CE1	HIS	C	66	80.633	14.699	43.095	1.00	43.67	C
ATOM	5041	NE2	HIS	C	66	79.379	14.305	43.221	1.00	42.62	C
ATOM	5042	C	HIS	C	66	80.823	18.750	43.544	1.00	46.51	C
ATOM	5043	O	HIS	C	66	81.063	18.025	44.505	1.00	47.99	C
ATOM	5044	N	HIS	C	67	81.781	19.393	42.894	1.00	47.66	C
ATOM	5045	CA	HIS	C	67	83.163	19.249	43.321	1.00	49.37	C
ATOM	5046	CB	HIS	C	67	84.059	18.952	42.127	1.00	50.68	C
ATOM	5047	CG	HIS	C	67	83.964	17.541	41.652	1.00	52.46	C
ATOM	5048	CD2	HIS	C	67	83.878	16.378	42.337	1.00	53.35	C
ATOM	5049	ND1	HIS	C	67	83.926	17.205	40.318	1.00	54.03	C
ATOM	5050	CE1	HIS	C	67	83.815	15.894	40.199	1.00	53.47	C
ATOM	5051	NE2	HIS	C	67	83.783	15.369	41.410	1.00	54.73	C
ATOM	5052	C	HIS	C	67	83.634	20.496	44.013	1.00	50.00	C
ATOM	5053	O	HIS	C	67	84.831	20.793	44.022	1.00	49.65	C
ATOM	5054	N	ARG	C	68	82.685	21.219	44.603	1.00	50.89	C
ATOM	5055	CA	ARG	C	68	82.996	22.468	45.295	1.00	52.52	C
ATOM	5056	CB	ARG	C	68	81.721	23.137	45.804	1.00	51.55	C
ATOM	5057	CG	ARG	C	68	80.882	22.281	46.708	1.00	51.00	C
ATOM	5058	CD	ARG	C	68	79.609	23.021	47.114	1.00	51.32	C
ATOM	5059	NE	ARG	C	68	78.436	22.163	46.984	1.00	50.65	C
ATOM	5060	CZ	ARG	C	68	78.319	20.978	47.571	1.00	49.83	C
ATOM	5061	NH1	ARG	C	68	79.299	20.514	48.331	1.00	53.30	C
ATOM	5062	NH2	ARG	C	68	77.232	20.249	47.391	1.00	50.27	C
ATOM	5063	C	ARG	C	68	83.967	22.310	46.442	1.00	53.96	C
ATOM	5064	O	ARG	C	68	84.685	23.243	46.784	1.00	54.35	C
ATOM	5065	N	ASP	C	69	83.993	21.134	47.046	1.00	56.66	C
ATOM	5066	CA	ASP	C	69	84.905	20.921	48.150	1.00	59.49	C
ATOM	5067	CB	ASP	C	69	84.147	20.357	49.361	1.00	58.83	C
ATOM	5068	CG	ASP	C	69	82.957	21.232	49.774	1.00	58.82	C
ATOM	5069	OD1	ASP	C	69	83.161	22.430	50.067	1.00	57.19	C
ATOM	5070	OD2	ASP	C	69	81.814	20.718	49.806	1.00	58.80	C
ATOM	5071	C	ASP	C	69	86.032	19.986	47.722	1.00	61.81	C
ATOM	5072	O	ASP	C	69	87.029	19.849	48.426	1.00	64.04	C
ATOM	5073	N	SER	C	70	85.890	19.355	46.561	1.00	62.80	C

```
ATOM   5074  CA  SER C  70      86.928  18.445  46.089  1.00 63.95      C
ATOM   5075  CB  SER C  70      86.501  17.796  44.777  1.00 64.08      C
ATOM   5076  OG  SER C  70      85.355  16.996  44.990  1.00 65.02      C
ATOM   5077  C   SER C  70      88.264  19.161  45.914  1.00 64.84      C
ATOM   5078  O   SER C  70      88.305  20.371  45.697  1.00 65.35      C
ATOM   5079  N   ASN C  71      89.360  18.418  46.029  1.00 65.33      C
ATOM   5080  CA  ASN C  71      90.678  19.015  45.878  1.00 65.77      C
ATOM   5081  CB  ASN C  71      91.549  18.684  47.091  1.00 67.38      C
ATOM   5082  CG  ASN C  71      90.805  18.874  48.409  1.00 70.03      C
ATOM   5083  OD1 ASN C  71      90.234  19.943  48.673  1.00 70.29      C
ATOM   5084  ND2 ASN C  71      90.807  17.832  49.246  1.00 70.86      C
ATOM   5085  C   ASN C  71      91.311  18.488  44.603  1.00 65.48      C
ATOM   5086  O   ASN C  71      91.311  17.280  44.351  1.00 65.01      C
ATOM   5087  N   PHE C  72      91.830  19.404  43.792  1.00 64.80      C
ATOM   5088  CA  PHE C  72      92.463  19.045  42.529  1.00 64.53      C
ATOM   5089  CB  PHE C  72      91.585  19.473  41.342  1.00 60.50      C
ATOM   5090  CG  PHE C  72      90.272  18.736  41.247  1.00 55.74      C
ATOM   5091  CD1 PHE C  72      89.068  19.433  41.235  1.00 53.23      C
ATOM   5092  CD2 PHE C  72      90.238  17.349  41.154  1.00 52.78      C
ATOM   5093  CE1 PHE C  72      87.856  18.758  41.127  1.00 51.24      C
ATOM   5094  CE2 PHE C  72      89.027  16.672  41.047  1.00 50.62      C
ATOM   5095  CZ  PHE C  72      87.837  17.378  41.034  1.00 50.12      C
ATOM   5096  C   PHE C  72      93.818  19.728  42.417  1.00 66.62      C
ATOM   5097  O   PHE C  72      93.940  20.918  42.709  1.00 67.09      C
ATOM   5098  N   PRO C  73      94.853  18.981  41.988  1.00 68.12      C
ATOM   5099  CD  PRO C  73      94.775  17.557  41.611  1.00 68.63      C
ATOM   5100  CA  PRO C  73      96.220  19.493  41.823  1.00 68.91      C
ATOM   5101  CB  PRO C  73      96.935  18.342  41.118  1.00 69.55      C
ATOM   5102  CG  PRO C  73      96.219  17.133  41.636  1.00 69.28      C
ATOM   5103  C   PRO C  73      96.257  20.778  40.990  1.00 69.17      C
ATOM   5104  O   PRO C  73      96.598  21.853  41.487  1.00 69.84      C
ATOM   5105  N   VAL C  86      90.900   7.286  36.371  1.00 88.13      C
ATOM   5106  CA  VAL C  86      90.597   6.804  37.711  1.00 88.42      C
ATOM   5107  CB  VAL C  86      91.894   6.677  38.553  1.00 87.81      C
ATOM   5108  CG1 VAL C  86      92.562   5.342  38.273  0.00 87.97      C
ATOM   5109  CG2 VAL C  86      92.855   7.813  38.214  1.00 86.72      C
ATOM   5110  C   VAL C  86      89.573   7.685  38.445  1.00 88.62      C
ATOM   5111  O   VAL C  86      89.901   8.362  39.423  1.00 88.93      C
ATOM   5112  N   ASP C  87      88.328   7.661  37.964  1.00 88.31      C
ATOM   5113  CA  ASP C  87      87.230   8.443  38.547  1.00 87.51      C
ATOM   5114  CB  ASP C  87      86.568   9.310  37.475  0.00 88.63      C
ATOM   5115  CG  ASP C  87      87.538  10.229  36.783  1.00 89.65      C
ATOM   5116  OD1 ASP C  87      87.832  11.313  37.331  1.00 90.42      C
ATOM   5117  OD2 ASP C  87      88.011   9.859  35.688  1.00 89.70      C
ATOM   5118  C   ASP C  87      86.150   7.559  39.166  1.00 86.41      C
ATOM   5119  O   ASP C  87      86.396   6.413  39.543  0.00 86.24      C
ATOM   5120  N   SER C  88      84.944   8.110  39.245  1.00 84.26      C
ATOM   5121  CA  SER C  88      83.803   7.402  39.800  1.00 82.05      C
ATOM   5122  CB  SER C  88      83.872   7.398  41.324  1.00 81.81      C
ATOM   5123  OG  SER C  88      82.634   6.987  41.874  1.00 81.31      C
ATOM   5124  C   SER C  88      82.508   8.067  39.360  1.00 80.69      C
ATOM   5125  O   SER C  88      81.919   7.704  38.342  1.00 81.28      C
ATOM   5126  N   TRP C  89      82.066   9.042  40.144  1.00 77.91      C
ATOM   5127  CA  TRP C  89      80.848   9.780  39.848  1.00 74.10      C
```

```
ATOM   5128  CB  TRP C  89      80.646  10.859  40.905  1.00 73.48      C
ATOM   5129  CG  TRP C  89      79.446  11.708  40.702  1.00 72.20      C
ATOM   5130  CD2 TRP C  89      79.428  13.044  40.197  1.00 71.86      C
ATOM   5131  CE2 TRP C  89      78.088  13.476  40.209  1.00 71.45      C
ATOM   5132  CE3 TRP C  89      80.418  13.919  39.735  1.00 71.66      C
ATOM   5133  CD1 TRP C  89      78.153  11.388  40.988  1.00 71.28      C
ATOM   5134  NE1 TRP C  89      77.329  12.446  40.698  1.00 70.67      C
ATOM   5135  CZ2 TRP C  89      77.711  14.750  39.780  1.00 71.55      C
ATOM   5136  CZ3 TRP C  89      80.043  15.184  39.308  1.00 71.26      C
ATOM   5137  CH2 TRP C  89      78.701  15.587  39.334  1.00 71.21      C
ATOM   5138  C   TRP C  89      80.995  10.415  38.473  1.00 72.28      C
ATOM   5139  O   TRP C  89      80.021  10.567  37.740  1.00 72.30      C
ATOM   5140  N   ASP C  90      82.229  10.779  38.136  1.00 70.00      C
ATOM   5141  CA  ASP C  90      82.543  11.389  36.848  1.00 67.79      C
ATOM   5142  CB  ASP C  90      84.011  11.810  36.808  1.00 64.52      C
ATOM   5143  CG  ASP C  90      84.300  13.010  37.685  1.00 61.24      C
ATOM   5144  OD1 ASP C  90      83.453  13.363  38.530  1.00 59.13      C
ATOM   5145  OD2 ASP C  90      85.388  13.594  37.533  1.00 58.53      C
ATOM   5146  C   ASP C  90      82.261  10.436  35.691  1.00 67.74      C
ATOM   5147  O   ASP C  90      81.888  10.868  34.597  1.00 68.39      C
ATOM   5148  N   ARG C  91      82.460   9.142  35.926  1.00 67.23      C
ATOM   5149  CA  ARG C  91      82.197   8.140  34.895  1.00 66.43      C
ATOM   5150  CB  ARG C  91      82.671   6.755  35.345  0.00 67.74      C
ATOM   5151  CG  ARG C  91      82.250   5.602  34.429  0.00 69.73      C
ATOM   5152  CD  ARG C  91      82.769   5.731  32.997  0.00 71.43      C
ATOM   5153  NE  ARG C  91      81.880   6.509  32.132  1.00 73.30      C
ATOM   5154  CZ  ARG C  91      81.888   6.448  30.803  1.00 73.96      C
ATOM   5155  NH1 ARG C  91      82.739   5.645  30.176  1.00 75.13      C
ATOM   5156  NH2 ARG C  91      81.038   7.180  30.098  1.00 73.71      C
ATOM   5157  C   ARG C  91      80.707   8.091  34.580  1.00 64.28      C
ATOM   5158  O   ARG C  91      80.322   8.005  33.416  1.00 64.65      C
ATOM   5159  N   GLU C  92      79.871   8.156  35.611  1.00 61.21      C
ATOM   5160  CA  GLU C  92      78.434   8.111  35.398  1.00 59.24      C
ATOM   5161  CB  GLU C  92      77.709   7.733  36.691  1.00 61.28      C
ATOM   5162  CG  GLU C  92      76.200   7.577  36.529  1.00 63.29      C
ATOM   5163  CD  GLU C  92      75.816   6.698  35.345  1.00 64.91      C
ATOM   5164  OE1 GLU C  92      76.430   5.618  35.171  1.00 65.27      C
ATOM   5165  OE2 GLU C  92      74.888   7.087  34.599  1.00 65.86      C
ATOM   5166  C   GLU C  92      77.947   9.463  34.908  1.00 56.10      C
ATOM   5167  O   GLU C  92      76.846   9.587  34.379  1.00 55.26      C
ATOM   5168  N   PHE C  93      78.786  10.473  35.088  1.00 52.97      C
ATOM   5169  CA  PHE C  93      78.470  11.828  34.669  1.00 49.46      C
ATOM   5170  CB  PHE C  93      79.271  12.821  35.504  1.00 47.72      C
ATOM   5171  CG  PHE C  93      79.168  14.237  35.031  1.00 46.31      C
ATOM   5172  CD1 PHE C  93      77.975  14.936  35.134  1.00 46.80      C
ATOM   5173  CD2 PHE C  93      80.274  14.880  34.487  1.00 46.30      C
ATOM   5174  CE1 PHE C  93      77.881  16.260  34.698  1.00 46.57      C
ATOM   5175  CE2 PHE C  93      80.194  16.200  34.048  1.00 45.89      C
ATOM   5176  CZ  PHE C  93      78.995  16.891  34.155  1.00 46.39      C
ATOM   5177  C   PHE C  93      78.805  12.007  33.195  1.00 48.24      C
ATOM   5178  O   PHE C  93      78.194  12.829  32.512  1.00 48.29      C
ATOM   5179  N   LEU C  94      79.777  11.241  32.706  1.00 46.95      C
ATOM   5180  CA  LEU C  94      80.181  11.334  31.304  1.00 46.69      C
ATOM   5181  CB  LEU C  94      81.711  11.421  31.201  1.00 43.72      C
```

```
ATOM   5182  CG  LEU C  94      82.347  12.602  31.931  1.00 42.20      C
ATOM   5183  CD1 LEU C  94      83.827  12.571  31.708  1.00 42.01      C
ATOM   5184  CD2 LEU C  94      81.761  13.918  31.444  1.00 40.79      C
ATOM   5185  C   LEU C  94      79.657  10.163  30.470  1.00 46.61      C
ATOM   5186  O   LEU C  94      80.084   9.950  29.331  1.00 47.53      C
ATOM   5187  N   LYS C  95      78.721   9.416  31.044  1.00 46.24      C
ATOM   5188  CA  LYS C  95      78.123   8.260  30.382  1.00 46.42      C
ATOM   5189  CB  LYS C  95      77.447   7.372  31.436  1.00 48.23      C
ATOM   5190  CG  LYS C  95      77.259   5.915  31.045  1.00 48.85      C
ATOM   5191  CD  LYS C  95      75.858   5.649  30.493  1.00 50.94      C
ATOM   5192  CE  LYS C  95      74.749   5.845  31.556  1.00 51.20      C
ATOM   5193  NZ  LYS C  95      74.537   7.259  32.014  1.00 49.42      C
ATOM   5194  C   LYS C  95      77.103   8.758  29.359  1.00 45.40      C
ATOM   5195  O   LYS C  95      76.000   8.222  29.234  1.00 45.79      C
ATOM   5196  N   VAL C  96      77.495   9.797  28.631  1.00 42.97      C
ATOM   5197  CA  VAL C  96      76.648  10.418  27.627  1.00 39.32      C
ATOM   5198  CB  VAL C  96      76.748  11.930  27.759  1.00 38.19      C
ATOM   5199  CG1 VAL C  96      76.296  12.335  29.143  1.00 37.83      C
ATOM   5200  CG2 VAL C  96      78.182  12.369  27.543  1.00 37.61      C
ATOM   5201  C   VAL C  96      77.069   9.973  26.224  1.00 39.45      C
ATOM   5202  O   VAL C  96      77.934   9.110  26.077  1.00 39.51      C
ATOM   5203  N   ASP C  97      76.448  10.545  25.197  1.00 38.96      C
ATOM   5204  CA  ASP C  97      76.776  10.194  23.820  1.00 38.45      C
ATOM   5205  CB  ASP C  97      75.596  10.485  22.907  1.00 40.12      C
ATOM   5206  CG  ASP C  97      75.212  11.951  22.907  1.00 41.57      C
ATOM   5207  OD1 ASP C  97      76.061  12.785  23.289  1.00 41.15      C
ATOM   5208  OD2 ASP C  97      74.066  12.271  22.516  1.00 42.19      C
ATOM   5209  C   ASP C  97      77.986  10.982  23.328  1.00 38.55      C
ATOM   5210  O   ASP C  97      78.331  12.014  23.893  1.00 37.77      C
ATOM   5211  N   GLN C  98      78.612  10.505  22.259  1.00 39.05      C
ATOM   5212  CA  GLN C  98      79.794  11.157  21.717  1.00 38.40      C
ATOM   5213  CB  GLN C  98      80.225  10.485  20.415  1.00 38.10      C
ATOM   5214  CG  GLN C  98      80.605   9.023  20.544  1.00 36.09      C
ATOM   5215  CD  GLN C  98      81.275   8.497  19.298  1.00 36.91      C
ATOM   5216  OE1 GLN C  98      81.239   9.130  18.236  1.00 36.92      C
ATOM   5217  NE2 GLN C  98      81.881   7.324  19.412  1.00 36.42      C
ATOM   5218  C   GLN C  98      79.650  12.653  21.470  1.00 39.08      C
ATOM   5219  O   GLN C  98      80.599  13.401  21.692  1.00 40.00      C
ATOM   5220  N   GLU C  99      78.486  13.088  21.001  1.00 39.22      C
ATOM   5221  CA  GLU C  99      78.271  14.502  20.726  1.00 40.50      C
ATOM   5222  CB  GLU C  99      76.891  14.717  20.126  1.00 42.47      C
ATOM   5223  CG  GLU C  99      76.918  15.343  18.756  1.00 45.54      C
ATOM   5224  CD  GLU C  99      77.806  16.577  18.697  1.00 47.73      C
ATOM   5225  OE1 GLU C  99      77.552  17.541  19.462  1.00 47.01      C
ATOM   5226  OE2 GLU C  99      78.757  16.577  17.881  1.00 47.67      C
ATOM   5227  C   GLU C  99      78.387  15.335  21.990  1.00 41.46      C
ATOM   5228  O   GLU C  99      78.980  16.418  21.993  1.00 41.51      C
ATOM   5229  N   MSE C 100      77.788  14.831  23.061  1.00 41.97      C
ATOM   5230  CA  MSE C 100      77.818  15.518  24.335  1.00 41.69      C
ATOM   5231  CB  MSE C 100      76.885  14.824  25.333  1.00 45.69      C
ATOM   5232  CG  MSE C 100      76.914  15.403  26.735  1.00 51.76      C
ATOM   5233  SE  MSE C 100      76.090  17.140  26.925  1.00 62.68      C
ATOM   5234  CE  MSE C 100      77.565  18.303  26.510  1.00 57.90      C
ATOM   5235  C   MSE C 100      79.243  15.546  24.867  1.00 39.87      C
```

```
ATOM   5236  O   MSE C 100      79.810  16.626  25.037  1.00 39.79      C
ATOM   5237  N   LEU C 101      79.835  14.376  25.115  1.00 37.39      C
ATOM   5238  CA  LEU C 101      81.199  14.341  25.651  1.00 34.99      C
ATOM   5239  CB  LEU C 101      81.809  12.938  25.539  1.00 33.34      C
ATOM   5240  CG  LEU C 101      83.130  12.730  26.289  1.00 30.53      C
ATOM   5241  CD1 LEU C 101      82.896  12.845  27.780  1.00 31.52      C
ATOM   5242  CD2 LEU C 101      83.684  11.363  25.965  1.00 30.51      C
ATOM   5243  C   LEU C 101      82.067  15.347  24.904  1.00 34.53      C
ATOM   5244  O   LEU C 101      82.753  16.184  25.516  1.00 34.23      C
ATOM   5245  N   TYR C 102      82.011  15.274  23.577  1.00 31.29      C
ATOM   5246  CA  TYR C 102      82.770  16.179  22.716  1.00 28.61      C
ATOM   5247  CB  TYR C 102      82.335  15.955  21.258  1.00 27.71      C
ATOM   5248  CG  TYR C 102      82.876  16.976  20.288  1.00 26.47      C
ATOM   5249  CD1 TYR C 102      84.220  16.970  19.896  1.00 24.67      C
ATOM   5250  CE1 TYR C 102      84.708  17.930  19.005  1.00 23.69      C
ATOM   5251  CD2 TYR C 102      82.040  17.960  19.774  1.00 25.15      C
ATOM   5252  CE2 TYR C 102      82.505  18.913  18.899  1.00 23.80      C
ATOM   5253  CZ  TYR C 102      83.827  18.899  18.512  1.00 23.80      C
ATOM   5254  OH  TYR C 102      84.237  19.853  17.626  1.00 21.51      C
ATOM   5255  C   TYR C 102      82.572  17.659  23.131  1.00 27.38      C
ATOM   5256  O   TYR C 102      83.536  18.383  23.433  1.00 23.78      C
ATOM   5257  N   GLU C 103      81.314  18.092  23.155  1.00 28.53      C
ATOM   5258  CA  GLU C 103      80.979  19.462  23.532  1.00 29.26      C
ATOM   5259  CB  GLU C 103      79.483  19.706  23.342  1.00 30.52      C
ATOM   5260  CG  GLU C 103      79.063  19.574  21.888  1.00 33.75      C
ATOM   5261  CD  GLU C 103      77.781  20.318  21.565  1.00 36.95      C
ATOM   5262  OE1 GLU C 103      77.729  21.549  21.820  1.00 41.36      C
ATOM   5263  OE2 GLU C 103      76.832  19.682  21.053  1.00 35.81      C
ATOM   5264  C   GLU C 103      81.397  19.817  24.954  1.00 27.19      C
ATOM   5265  O   GLU C 103      81.801  20.950  25.217  1.00 27.16      C
ATOM   5266  N   ILE C 104      81.317  18.855  25.870  1.00 26.37      C
ATOM   5267  CA  ILE C 104      81.717  19.114  27.254  1.00 25.70      C
ATOM   5268  CB  ILE C 104      81.356  17.913  28.167  1.00 25.25      C
ATOM   5269  CG2 ILE C 104      82.091  17.986  29.485  1.00 25.29      C
ATOM   5270  CG1 ILE C 104      79.859  17.935  28.450  1.00 25.32      C
ATOM   5271  CD1 ILE C 104      79.346  16.709  29.127  1.00 25.12      C
ATOM   5272  C   ILE C 104      83.210  19.423  27.310  1.00 24.54      C
ATOM   5273  O   ILE C 104      83.614  20.452  27.848  1.00 22.76      C
ATOM   5274  N   ILE C 105      84.011  18.528  26.731  1.00 24.67      C
ATOM   5275  CA  ILE C 105      85.464  18.687  26.673  1.00 23.37      C
ATOM   5276  CB  ILE C 105      86.120  17.563  25.834  1.00 22.40      C
ATOM   5277  CG2 ILE C 105      87.524  17.985  25.410  1.00 22.41      C
ATOM   5278  CG1 ILE C 105      86.143  16.249  26.630  1.00 22.74      C
ATOM   5279  CD1 ILE C 105      86.616  15.035  25.826  1.00 19.84      C
ATOM   5280  C   ILE C 105      85.844  20.038  26.057  1.00 24.11      C
ATOM   5281  O   ILE C 105      86.885  20.601  26.383  1.00 23.21      C
ATOM   5282  N   LEU C 106      85.007  20.568  25.170  1.00 25.59      C
ATOM   5283  CA  LEU C 106      85.341  21.845  24.546  1.00 26.22      C
ATOM   5284  CB  LEU C 106      84.550  22.060  23.251  1.00 24.35      C
ATOM   5285  CG  LEU C 106      84.955  21.288  21.982  1.00 24.05      C
ATOM   5286  CD1 LEU C 106      84.041  21.702  20.824  1.00 19.50      C
ATOM   5287  CD2 LEU C 106      86.411  21.582  21.631  1.00 19.81      C
ATOM   5288  C   LEU C 106      85.051  22.972  25.504  1.00 27.00      C
ATOM   5289  O   LEU C 106      85.876  23.871  25.700  1.00 28.04      C
```

```
ATOM   5290  N   ALA C 107      83.870  22.908  26.107  1.00 27.32      C
ATOM   5291  CA  ALA C 107      83.432  23.921  27.054  1.00 27.07      C
ATOM   5292  CB  ALA C 107      82.044  23.574  27.562  1.00 27.09      C
ATOM   5293  C   ALA C 107      84.417  23.967  28.210  1.00 26.97      C
ATOM   5294  O   ALA C 107      84.759  25.040  28.720  1.00 25.71      C
ATOM   5295  N   ALA C 108      84.866  22.786  28.621  1.00 27.46      C
ATOM   5296  CA  ALA C 108      85.809  22.688  29.726  1.00 28.55      C
ATOM   5297  CB  ALA C 108      86.059  21.230  30.069  1.00 27.60      C
ATOM   5298  C   ALA C 108      87.119  23.383  29.363  1.00 29.01      C
ATOM   5299  O   ALA C 108      87.595  24.264  30.085  1.00 29.74      C
ATOM   5300  N   ASN C 109      87.684  22.988  28.227  1.00 28.31      C
ATOM   5301  CA  ASN C 109      88.934  23.554  27.723  1.00 27.27      C
ATOM   5302  CB  ASN C 109      89.213  22.988  26.323  1.00 27.05      C
ATOM   5303  CG  ASN C 109      90.436  23.594  25.666  1.00 24.65      C
ATOM   5304  OD1 ASN C 109      91.542  23.472  26.167  1.00 22.66      C
ATOM   5305  ND2 ASN C 109      90.236  24.235  24.517  1.00 24.60      C
ATOM   5306  C   ASN C 109      88.848  25.074  27.661  1.00 27.03      C
ATOM   5307  O   ASN C 109      89.755  25.770  28.109  1.00 28.21      C
ATOM   5308  N   TYR C 110      87.743  25.575  27.118  1.00 26.52      C
ATOM   5309  CA  TYR C 110      87.528  27.003  26.969  1.00 26.57      C
ATOM   5310  CB  TYR C 110      86.268  27.267  26.139  1.00 25.48      C
ATOM   5311  CG  TYR C 110      85.938  28.734  26.018  1.00 24.82      C
ATOM   5312  CD1 TYR C 110      86.780  29.596  25.317  1.00 26.81      C
ATOM   5313  CE1 TYR C 110      86.543  30.968  25.273  1.00 26.16      C
ATOM   5314  CD2 TYR C 110      84.838  29.282  26.669  1.00 24.41      C
ATOM   5315  CE2 TYR C 110      84.596  30.658  26.628  1.00 24.83      C
ATOM   5316  CZ  TYR C 110      85.455  31.486  25.930  1.00 24.87      C
ATOM   5317  OH  TYR C 110      85.234  32.835  25.889  1.00 25.53      C
ATOM   5318  C   TYR C 110      87.371  27.682  28.308  1.00 27.74      C
ATOM   5319  O   TYR C 110      87.907  28.767  28.546  1.00 27.37      C
ATOM   5320  N   LEU C 111      86.610  27.040  29.178  1.00 28.23      C
ATOM   5321  CA  LEU C 111      86.348  27.593  30.485  1.00 28.18      C
ATOM   5322  CB  LEU C 111      85.067  26.958  31.031  1.00 25.97      C
ATOM   5323  CG  LEU C 111      83.874  27.827  31.434  1.00 24.04      C
ATOM   5324  CD1 LEU C 111      83.755  29.132  30.657  1.00 19.70      C
ATOM   5325  CD2 LEU C 111      82.653  26.963  31.273  1.00 24.33      C
ATOM   5326  C   LEU C 111      87.547  27.373  31.410  1.00 29.42      C
ATOM   5327  O   LEU C 111      87.524  27.765  32.578  1.00 31.45      C
ATOM   5328  N   ASN C 112      88.601  26.761  30.875  1.00 29.81      C
ATOM   5329  CA  ASN C 112      89.825  26.513  31.640  1.00 31.10      C
ATOM   5330  CB  ASN C 112      90.498  27.835  32.006  1.00 31.09      C
ATOM   5331  CG  ASN C 112      91.974  27.673  32.371  1.00 32.09      C
ATOM   5332  OD1 ASN C 112      92.448  26.579  32.719  1.00 29.20      C
ATOM   5333  ND2 ASN C 112      92.708  28.783  32.300  1.00 33.07      C
ATOM   5334  C   ASN C 112      89.563  25.740  32.927  1.00 32.17      C
ATOM   5335  O   ASN C 112      89.805  26.237  34.030  1.00 33.29      C
ATOM   5336  N   ILE C 113      89.055  24.527  32.789  1.00 31.11      C
ATOM   5337  CA  ILE C 113      88.798  23.717  33.954  1.00 30.18      C
ATOM   5338  CB  ILE C 113      87.322  23.467  34.163  1.00 30.05      C
ATOM   5339  CG2 ILE C 113      87.131  22.660  35.442  1.00 28.92      C
ATOM   5340  CG1 ILE C 113      86.564  24.789  34.234  1.00 28.96      C
ATOM   5341  CD1 ILE C 113      85.076  24.575  34.283  1.00 28.52      C
ATOM   5342  C   ILE C 113      89.473  22.384  33.751  1.00 30.85      C
ATOM   5343  O   ILE C 113      88.834  21.400  33.387  1.00 29.72      C
```

```
ATOM   5344  N   LYS C 114      90.778  22.368  33.998  1.00 31.38      C
ATOM   5345  CA  LYS C 114      91.595  21.173  33.838  1.00 31.36      C
ATOM   5346  CB  LYS C 114      93.003  21.440  34.383  1.00 32.37      C
ATOM   5347  CG  LYS C 114      93.901  20.219  34.344  1.00 34.25      C
ATOM   5348  CD  LYS C 114      95.372  20.555  34.550  1.00 35.39      C
ATOM   5349  CE  LYS C 114      96.190  19.289  34.455  1.00 36.88      C
ATOM   5350  NZ  LYS C 114      95.863  18.587  33.190  1.00 40.06      C
ATOM   5351  C   LYS C 114      91.035  19.876  34.437  1.00 30.61      C
ATOM   5352  O   LYS C 114      91.054  18.841  33.785  1.00 30.70      C
ATOM   5353  N   PRO C 115      90.530  19.916  35.681  1.00 30.70      C
ATOM   5354  CD  PRO C 115      90.401  21.106  36.545  1.00 31.09      C
ATOM   5355  CA  PRO C 115      89.970  18.719  36.338  1.00 30.04      C
ATOM   5356  CB  PRO C 115      89.365  19.276  37.626  1.00 30.45      C
ATOM   5357  CG  PRO C 115      90.220  20.489  37.912  1.00 31.85      C
ATOM   5358  C   PRO C 115      88.914  18.030  35.482  1.00 29.80      C
ATOM   5359  O   PRO C 115      88.935  16.806  35.295  1.00 30.05      C
ATOM   5360  N   LEU C 116      87.981  18.833  34.974  1.00 29.91      C
ATOM   5361  CA  LEU C 116      86.904  18.330  34.114  1.00 29.38      C
ATOM   5362  CB  LEU C 116      85.797  19.376  33.980  1.00 27.77      C
ATOM   5363  CG  LEU C 116      84.628  18.909  33.138  1.00 27.38      C
ATOM   5364  CD1 LEU C 116      84.043  17.676  33.768  1.00 27.48      C
ATOM   5365  CD2 LEU C 116      83.597  20.023  33.027  1.00 27.97      C
ATOM   5366  C   LEU C 116      87.464  17.974  32.731  1.00 28.24      C
ATOM   5367  O   LEU C 116      87.042  17.003  32.107  1.00 28.34      C
ATOM   5368  N   LEU C 117      88.433  18.756  32.272  1.00 26.39      C
ATOM   5369  CA  LEU C 117      89.051  18.494  30.993  1.00 26.69      C
ATOM   5370  CB  LEU C 117      90.112  19.547  30.701  1.00 24.99      C
ATOM   5371  CG  LEU C 117      90.893  19.362  29.397  1.00 24.42      C
ATOM   5372  CD1 LEU C 117      89.943  19.112  28.225  1.00 23.60      C
ATOM   5373  CD2 LEU C 117      91.738  20.593  29.154  1.00 22.70      C
ATOM   5374  C   LEU C 117      89.680  17.100  30.981  1.00 28.34      C
ATOM   5375  O   LEU C 117      89.397  16.288  30.093  1.00 29.22      C
ATOM   5376  N   ASP C 118      90.528  16.826  31.973  1.00 29.30      C
ATOM   5377  CA  ASP C 118      91.207  15.532  32.105  1.00 29.52      C
ATOM   5378  CB  ASP C 118      92.117  15.538  33.347  1.00 32.96      C
ATOM   5379  CG  ASP C 118      93.158  16.668  33.316  1.00 36.46      C
ATOM   5380  OD1 ASP C 118      93.138  17.470  32.353  1.00 37.36      C
ATOM   5381  OD2 ASP C 118      93.990  16.757  34.253  1.00 36.80      C
ATOM   5382  C   ASP C 118      90.213  14.365  32.186  1.00 28.84      C
ATOM   5383  O   ASP C 118      90.289  13.418  31.391  1.00 28.39      C
ATOM   5384  N   ALA C 119      89.288  14.419  33.142  1.00 26.34      C
ATOM   5385  CA  ALA C 119      88.293  13.348  33.262  1.00 25.58      C
ATOM   5386  CB  ALA C 119      87.208  13.741  34.258  1.00 26.08      C
ATOM   5387  C   ALA C 119      87.654  13.022  31.899  1.00 24.81      C
ATOM   5388  O   ALA C 119      87.489  11.852  31.540  1.00 23.57      C
ATOM   5389  N   GLY C 120      87.282  14.060  31.154  1.00 22.99      C
ATOM   5390  CA  GLY C 120      86.695  13.840  29.850  1.00 23.36      C
ATOM   5391  C   GLY C 120      87.654  13.095  28.932  1.00 23.32      C
ATOM   5392  O   GLY C 120      87.284  12.124  28.282  1.00 22.39      C
ATOM   5393  N   CYS C 121      88.902  13.541  28.901  1.00 23.17      C
ATOM   5394  CA  CYS C 121      89.918  12.935  28.065  1.00 23.66      C
ATOM   5395  CB  CYS C 121      91.184  13.762  28.144  1.00 24.22      C
ATOM   5396  SG  CYS C 121      90.981  15.370  27.390  1.00 31.59      C
ATOM   5397  C   CYS C 121      90.215  11.497  28.425  1.00 24.08      C
```

```
ATOM   5398  O   CYS C 121      90.601  10.703  27.570  1.00 25.40      C
ATOM   5399  N   LYS C 122      90.026  11.155  29.692  1.00 25.04      C
ATOM   5400  CA  LYS C 122      90.270   9.796  30.138  1.00 24.59      C
ATOM   5401  CB  LYS C 122      90.293   9.740  31.672  1.00 25.68      C
ATOM   5402  CG  LYS C 122      91.396  10.599  32.270  1.00 26.14      C
ATOM   5403  CD  LYS C 122      91.580  10.400  33.763  1.00 27.91      C
ATOM   5404  CE  LYS C 122      92.594  11.421  34.315  1.00 29.43      C
ATOM   5405  NZ  LYS C 122      93.121  11.095  35.679  1.00 31.16      C
ATOM   5406  C   LYS C 122      89.179   8.897  29.571  1.00 24.85      C
ATOM   5407  O   LYS C 122      89.451   7.798  29.080  1.00 24.38      C
ATOM   5408  N   VAL C 123      87.940   9.366  29.611  1.00 26.05      C
ATOM   5409  CA  VAL C 123      86.856   8.555  29.071  1.00 27.70      C
ATOM   5410  CB  VAL C 123      85.509   9.274  29.197  1.00 28.31      C
ATOM   5411  CG1 VAL C 123      84.389   8.383  28.667  1.00 28.23      C
ATOM   5412  CG2 VAL C 123      85.272   9.627  30.650  1.00 26.87      C
ATOM   5413  C   VAL C 123      87.142   8.223  27.606  1.00 27.72      C
ATOM   5414  O   VAL C 123      86.946   7.083  27.165  1.00 27.83      C
ATOM   5415  N   VAL C 124      87.618   9.212  26.855  1.00 27.26      C
ATOM   5416  CA  VAL C 124      87.947   8.982  25.452  1.00 27.88      C
ATOM   5417  CB  VAL C 124      88.458  10.274  24.776  1.00 26.84      C
ATOM   5418  CG1 VAL C 124      88.953   9.959  23.368  1.00 26.47      C
ATOM   5419  CG2 VAL C 124      87.322  11.304  24.713  1.00 23.58      C
ATOM   5420  C   VAL C 124      89.008   7.880  25.343  1.00 28.21      C
ATOM   5421  O   VAL C 124      88.830   6.898  24.599  1.00 27.09      C
ATOM   5422  N   ALA C 125      90.097   8.041  26.095  1.00 26.95      C
ATOM   5423  CA  ALA C 125      91.170   7.050  26.102  1.00 29.33      C
ATOM   5424  CB  ALA C 125      92.268   7.479  27.044  1.00 27.76      C
ATOM   5425  C   ALA C 125      90.653   5.661  26.501  1.00 31.95      C
ATOM   5426  O   ALA C 125      91.063   4.647  25.930  1.00 32.25      C
ATOM   5427  N   GLU C 126      89.749   5.617  27.476  1.00 34.71      C
ATOM   5428  CA  GLU C 126      89.179   4.356  27.919  1.00 36.70      C
ATOM   5429  CB  GLU C 126      88.333   4.572  29.173  1.00 39.48      C
ATOM   5430  CG  GLU C 126      87.803   3.290  29.782  1.00 45.29      C
ATOM   5431  CD  GLU C 126      88.919   2.320  30.166  1.00 50.81      C
ATOM   5432  OE1 GLU C 126      89.934   2.813  30.740  1.00 52.04      C
ATOM   5433  OE2 GLU C 126      88.780   1.083  29.904  1.00 50.45      C
ATOM   5434  C   GLU C 126      88.325   3.739  26.813  1.00 35.98      C
ATOM   5435  O   GLU C 126      87.849   2.628  26.968  1.00 33.64      C
ATOM   5436  N   MSE C 127      88.123   4.477  25.717  1.00 37.74      C
ATOM   5437  CA  MSE C 127      87.355   3.994  24.563  1.00 39.73      C
ATOM   5438  CB  MSE C 127      86.592   5.129  23.866  1.00 41.63      C
ATOM   5439  CG  MSE C 127      85.526   5.848  24.700  1.00 42.19      C
ATOM   5440  SE  MSE C 127      84.412   7.110  23.629  1.00 43.57      C
ATOM   5441  CE  MSE C 127      82.969   5.916  23.133  1.00 43.96      C
ATOM   5442  C   MSE C 127      88.295   3.377  23.530  1.00 40.34      C
ATOM   5443  O   MSE C 127      87.885   2.517  22.753  1.00 41.30      C
ATOM   5444  N   ILE C 128      89.544   3.835  23.506  1.00 40.42      C
ATOM   5445  CA  ILE C 128      90.516   3.309  22.559  1.00 39.85      C
ATOM   5446  CB  ILE C 128      91.552   4.378  22.130  1.00 39.70      C
ATOM   5447  CG2 ILE C 128      92.689   3.746  21.349  1.00 39.51      C
ATOM   5448  CG1 ILE C 128      90.879   5.426  21.254  1.00 38.45      C
ATOM   5449  CD1 ILE C 128      90.118   6.401  22.035  1.00 40.80      C
ATOM   5450  C   ILE C 128      91.245   2.174  23.224  1.00 39.58      C
ATOM   5451  O   ILE C 128      91.534   1.156  22.603  1.00 40.22      C
```

```
ATOM   5452  N   ARG C 129      91.518   2.353  24.508  1.00 39.78      C
ATOM   5453  CA  ARG C 129      92.230   1.362  25.300  1.00 38.47      C
ATOM   5454  CB  ARG C 129      91.959   1.599  26.781  1.00 39.40      C
ATOM   5455  CG  ARG C 129      93.052   1.083  27.689  1.00 38.81      C
ATOM   5456  CD  ARG C 129      92.731   1.379  29.130  1.00 40.09      C
ATOM   5457  NE  ARG C 129      92.640   2.812  29.456  1.00 42.40      C
ATOM   5458  CZ  ARG C 129      93.651   3.680  29.437  1.00 41.54      C
ATOM   5459  NH1 ARG C 129      94.869   3.283  29.089  1.00 41.83      C
ATOM   5460  NH2 ARG C 129      93.443   4.937  29.815  1.00 39.32      C
ATOM   5461  C   ARG C 129      91.863  -0.066  24.940  1.00 37.14      C
ATOM   5462  O   ARG C 129      90.682  -0.428  24.875  1.00 34.49      C
ATOM   5463  N   GLY C 130      92.900  -0.860  24.688  1.00 36.58      C
ATOM   5464  CA  GLY C 130      92.732  -2.264  24.356  1.00 36.84      C
ATOM   5465  C   GLY C 130      92.098  -2.656  23.032  1.00 36.85      C
ATOM   5466  O   GLY C 130      92.210  -3.816  22.626  1.00 37.50      C
ATOM   5467  N   ARG C 131      91.431  -1.721  22.359  1.00 37.11      C
ATOM   5468  CA  ARG C 131      90.787  -2.017  21.073  1.00 37.10      C
ATOM   5469  CB  ARG C 131      89.711  -0.973  20.771  1.00 39.22      C
ATOM   5470  CG  ARG C 131      88.431  -1.131  21.569  1.00 41.84      C
ATOM   5471  CD  ARG C 131      87.839  -2.509  21.363  1.00 45.09      C
ATOM   5472  NE  ARG C 131      86.396  -2.558  21.604  1.00 47.90      C
ATOM   5473  CZ  ARG C 131      85.479  -2.055  20.780  1.00 49.21      C
ATOM   5474  NH1 ARG C 131      85.846  -1.459  19.656  1.00 49.53      C
ATOM   5475  NH2 ARG C 131      84.191  -2.155  21.073  1.00 51.64      C
ATOM   5476  C   ARG C 131      91.760  -2.084  19.894  1.00 35.38      C
ATOM   5477  O   ARG C 131      92.917  -1.676  19.989  1.00 34.16      C
ATOM   5478  N   SER C 132      91.277  -2.610  18.781  1.00 33.40      C
ATOM   5479  CA  SER C 132      92.093  -2.717  17.585  1.00 32.90      C
ATOM   5480  CB  SER C 132      91.933  -4.096  16.966  1.00 31.03      C
ATOM   5481  OG  SER C 132      90.581  -4.307  16.607  1.00 31.69      C
ATOM   5482  C   SER C 132      91.646  -1.661  16.576  1.00 32.11      C
ATOM   5483  O   SER C 132      90.585  -1.054  16.738  1.00 30.91      C
ATOM   5484  N   PRO C 133      92.462  -1.422  15.532  1.00 31.16      C
ATOM   5485  CD  PRO C 133      93.848  -1.900  15.407  1.00 29.35      C
ATOM   5486  CA  PRO C 133      92.180  -0.451  14.480  1.00 32.65      C
ATOM   5487  CB  PRO C 133      93.219  -0.801  13.441  1.00 29.52      C
ATOM   5488  CG  PRO C 133      94.400  -1.021  14.307  1.00 29.23      C
ATOM   5489  C   PRO C 133      90.754  -0.514  13.963  1.00 35.83      C
ATOM   5490  O   PRO C 133      90.054   0.504  13.909  1.00 36.35      C
ATOM   5491  N   GLU C 134      90.318  -1.709  13.588  1.00 38.45      C
ATOM   5492  CA  GLU C 134      88.962  -1.875  13.104  1.00 41.11      C
ATOM   5493  CB  GLU C 134      88.765  -3.265  12.494  1.00 44.05      C
ATOM   5494  CG  GLU C 134      88.697  -3.264  10.965  1.00 49.94      C
ATOM   5495  CD  GLU C 134      87.779  -2.177  10.405  1.00 52.39      C
ATOM   5496  OE1 GLU C 134      86.664  -2.011  10.958  1.00 54.43      C
ATOM   5497  OE2 GLU C 134      88.173  -1.503   9.413  1.00 51.18      C
ATOM   5498  C   GLU C 134      87.968  -1.660  14.249  1.00 41.19      C
ATOM   5499  O   GLU C 134      86.913  -1.040  14.062  1.00 40.64      C
ATOM   5500  N   GLU C 135      88.297  -2.162  15.437  1.00 41.33      C
ATOM   5501  CA  GLU C 135      87.399  -1.978  16.575  1.00 42.01      C
ATOM   5502  CB  GLU C 135      87.915  -2.697  17.820  1.00 42.98      C
ATOM   5503  CG  GLU C 135      87.961  -4.198  17.745  1.00 44.16      C
ATOM   5504  CD  GLU C 135      88.393  -4.796  19.073  1.00 46.95      C
ATOM   5505  OE1 GLU C 135      89.419  -4.323  19.629  1.00 46.77      C
```

```
ATOM   5506  OE2 GLU C 135      87.712  -5.728  19.565  1.00 48.28      C
ATOM   5507  C   GLU C 135      87.226  -0.489  16.908  1.00 40.82      C
ATOM   5508  O   GLU C 135      86.152  -0.055  17.328  1.00 42.69      C
ATOM   5509  N   ILE C 136      88.284   0.292  16.718  1.00 37.69      C
ATOM   5510  CA  ILE C 136      88.224   1.718  16.997  1.00 33.59      C
ATOM   5511  CB  ILE C 136      89.638   2.316  17.096  1.00 32.05      C
ATOM   5512  CG2 ILE C 136      89.552   3.838  17.349  1.00 27.02      C
ATOM   5513  CG1 ILE C 136      90.412   1.564  18.196  1.00 29.01      C
ATOM   5514  CD1 ILE C 136      91.859   1.992  18.390  1.00 26.23      C
ATOM   5515  C   ILE C 136      87.442   2.419  15.903  1.00 33.18      C
ATOM   5516  O   ILE C 136      86.631   3.299  16.171  1.00 31.83      C
ATOM   5517  N   ARG C 137      87.669   2.021  14.661  1.00 34.42      C
ATOM   5518  CA  ARG C 137      86.955   2.652  13.566  1.00 34.64      C
ATOM   5519  CB  ARG C 137      87.352   2.008  12.253  1.00 33.73      C
ATOM   5520  CG  ARG C 137      88.809   2.218  11.916  1.00 34.55      C
ATOM   5521  CD  ARG C 137      89.226   1.238  10.851  1.00 34.62      C
ATOM   5522  NE  ARG C 137      90.665   1.216  10.644  1.00 33.99      C
ATOM   5523  CZ  ARG C 137      91.340   0.120  10.328  1.00 34.12      C
ATOM   5524  NH1 ARG C 137      90.694  -1.029  10.197  1.00 32.84      C
ATOM   5525  NH2 ARG C 137      92.651   0.176  10.125  1.00 34.77      C
ATOM   5526  C   ARG C 137      85.454   2.549  13.774  1.00 35.03      C
ATOM   5527  O   ARG C 137      84.745   3.538  13.638  1.00 34.65      C
ATOM   5528  N   ARG C 138      84.968   1.366  14.132  1.00 35.13      C
ATOM   5529  CA  ARG C 138      83.539   1.211  14.328  1.00 36.00      C
ATOM   5530  CB  ARG C 138      83.176  -0.270  14.439  1.00 38.78      C
ATOM   5531  CG  ARG C 138      83.339  -1.037  13.114  1.00 43.46      C
ATOM   5532  CD  ARG C 138      82.329  -0.608  12.030  0.00 47.14      C
ATOM   5533  NE  ARG C 138      82.537   0.734  11.466  0.00 51.00      C
ATOM   5534  CZ  ARG C 138      83.462   1.061  10.563  1.00 54.05      C
ATOM   5535  NH1 ARG C 138      84.302   0.146  10.095  1.00 55.91      C
ATOM   5536  NH2 ARG C 138      83.532   2.307  10.105  1.00 54.20      C
ATOM   5537  C   ARG C 138      83.008   1.990  15.528  1.00 34.39      C
ATOM   5538  O   ARG C 138      81.816   2.264  15.626  1.00 34.40      C
ATOM   5539  N   THR C 139      83.895   2.377  16.426  1.00 31.97      C
ATOM   5540  CA  THR C 139      83.486   3.123  17.596  1.00 29.98      C
ATOM   5541  CB  THR C 139      84.575   3.077  18.624  1.00 30.24      C
ATOM   5542  OG1 THR C 139      84.946   1.713  18.825  1.00 31.86      C
ATOM   5543  CG2 THR C 139      84.120   3.697  19.923  1.00 28.26      C
ATOM   5544  C   THR C 139      83.214   4.573  17.265  1.00 29.86      C
ATOM   5545  O   THR C 139      82.267   5.180  17.767  1.00 30.37      C
ATOM   5546  N   PHE C 140      84.053   5.138  16.415  1.00 29.19      C
ATOM   5547  CA  PHE C 140      83.883   6.525  16.045  1.00 28.27      C
ATOM   5548  CB  PHE C 140      85.229   7.230  16.152  1.00 25.82      C
ATOM   5549  CG  PHE C 140      85.797   7.223  17.537  1.00 23.52      C
ATOM   5550  CD1 PHE C 140      85.228   7.990  18.543  1.00 22.27      C
ATOM   5551  CD2 PHE C 140      86.907   6.452  17.844  1.00 22.34      C
ATOM   5552  CE1 PHE C 140      85.767   7.982  19.839  1.00 20.23      C
ATOM   5553  CE2 PHE C 140      87.450   6.441  19.135  1.00 18.70      C
ATOM   5554  CZ  PHE C 140      86.880   7.204  20.126  1.00 17.04      C
ATOM   5555  C   PHE C 140      83.307   6.697  14.647  1.00 28.75      C
ATOM   5556  O   PHE C 140      83.087   7.822  14.221  1.00 30.09      C
ATOM   5557  N   ASN C 141      83.027   5.585  13.964  1.00 29.40      C
ATOM   5558  CA  ASN C 141      82.521   5.589  12.580  1.00 30.10      C
ATOM   5559  CB  ASN C 141      81.182   6.335  12.434  1.00 30.86      C
```

```
ATOM   5560  CG  ASN C 141      80.620   6.279  10.991  1.00 32.35      C
ATOM   5561  OD1 ASN C 141      80.549   5.206  10.385  1.00 30.84      C
ATOM   5562  ND2 ASN C 141      80.212   7.436  10.453  1.00 32.26      C
ATOM   5563  C   ASN C 141      83.554   6.256  11.680  1.00 30.32      C
ATOM   5564  O   ASN C 141      83.223   7.047  10.803  1.00 31.59      C
ATOM   5565  N   ILE C 142      84.821   5.953  11.907  1.00 29.73      C
ATOM   5566  CA  ILE C 142      85.867   6.548  11.091  1.00 30.11      C
ATOM   5567  CB  ILE C 142      87.151   6.830  11.983  1.00 29.75      C
ATOM   5568  CG2 ILE C 142      87.180   5.925  13.180  1.00 31.60      C
ATOM   5569  CG1 ILE C 142      88.428   6.712  11.164  1.00 29.84      C
ATOM   5570  CD1 ILE C 142      88.925   8.056  10.663  1.00 36.02      C
ATOM   5571  C   ILE C 142      86.129   5.630   9.885  1.00 28.78      C
ATOM   5572  O   ILE C 142      86.070   4.412  10.004  1.00 27.70      C
ATOM   5573  N   VAL C 143      86.355   6.201   8.708  1.00 28.81      C
ATOM   5574  CA  VAL C 143      86.594   5.344   7.556  1.00 28.92      C
ATOM   5575  CB  VAL C 143      86.022   5.937   6.250  1.00 27.33      C
ATOM   5576  CG1 VAL C 143      86.549   5.165   5.056  1.00 27.92      C
ATOM   5577  CG2 VAL C 143      84.494   5.866   6.269  1.00 26.26      C
ATOM   5578  C   VAL C 143      88.071   5.084   7.356  1.00 28.95      C
ATOM   5579  O   VAL C 143      88.905   5.971   7.539  1.00 31.52      C
ATOM   5580  N   ASN C 144      88.387   3.845   7.006  1.00 27.50      C
ATOM   5581  CA  ASN C 144      89.754   3.434   6.761  1.00 26.06      C
ATOM   5582  CB  ASN C 144      89.837   1.907   6.798  1.00 27.42      C
ATOM   5583  CG  ASN C 144      91.258   1.377   6.661  1.00 28.39      C
ATOM   5584  OD1 ASN C 144      91.528   0.242   7.035  1.00 28.70      C
ATOM   5585  ND2 ASN C 144      92.162   2.185   6.119  1.00 30.75      C
ATOM   5586  C   ASN C 144      90.074   3.942   5.371  1.00 26.48      C
ATOM   5587  O   ASN C 144      89.519   3.458   4.394  1.00 26.51      C
ATOM   5588  N   ASP C 145      90.964   4.918   5.277  1.00 26.34      C
ATOM   5589  CA  ASP C 145      91.315   5.492   3.988  1.00 27.61      C
ATOM   5590  CB  ASP C 145      91.245   7.018   4.058  1.00 28.15      C
ATOM   5591  CG  ASP C 145      91.840   7.570   5.336  1.00 28.20      C
ATOM   5592  OD1 ASP C 145      92.508   6.808   6.080  1.00 26.63      C
ATOM   5593  OD2 ASP C 145      91.639   8.780   5.595  1.00 29.52      C
ATOM   5594  C   ASP C 145      92.684   5.086   3.479  1.00 28.92      C
ATOM   5595  O   ASP C 145      93.208   5.708   2.549  1.00 29.06      C
ATOM   5596  N   PHE C 146      93.262   4.050   4.083  1.00 28.68      C
ATOM   5597  CA  PHE C 146      94.585   3.572   3.685  1.00 29.48      C
ATOM   5598  CB  PHE C 146      95.222   2.744   4.799  1.00 31.05      C
ATOM   5599  CG  PHE C 146      95.709   3.550   5.955  1.00 33.63      C
ATOM   5600  CD1 PHE C 146      96.641   4.574   5.761  1.00 34.53      C
ATOM   5601  CD2 PHE C 146      95.277   3.254   7.250  1.00 33.58      C
ATOM   5602  CE1 PHE C 146      97.147   5.292   6.841  1.00 35.14      C
ATOM   5603  CE2 PHE C 146      95.767   3.956   8.338  1.00 34.74      C
ATOM   5604  CZ  PHE C 146      96.709   4.981   8.136  1.00 36.19      C
ATOM   5605  C   PHE C 146      94.596   2.727   2.431  1.00 28.86      C
ATOM   5606  O   PHE C 146      93.889   1.725   2.355  1.00 30.57      C
ATOM   5607  N   THR C 147      95.423   3.109   1.460  1.00 28.83      C
ATOM   5608  CA  THR C 147      95.536   2.339   0.222  1.00 30.01      C
ATOM   5609  CB  THR C 147      96.556   2.946  -0.783  1.00 29.36      C
ATOM   5610  OG1 THR C 147      97.817   3.147  -0.128  1.00 29.97      C
ATOM   5611  CG2 THR C 147      96.046   4.252  -1.355  1.00 27.00      C
ATOM   5612  C   THR C 147      96.049   0.948   0.552  1.00 30.37      C
ATOM   5613  O   THR C 147      96.708   0.745   1.563  1.00 31.13      C
```

```
ATOM   5614  N   PRO C 148      95.751  -0.032  -0.299  1.00 31.61      C
ATOM   5615  CD  PRO C 148      94.879  -0.031  -1.485  1.00 31.67      C
ATOM   5616  CA  PRO C 148      96.241  -1.375  -0.010  1.00 32.60      C
ATOM   5617  CB  PRO C 148      95.903  -2.141  -1.282  1.00 31.26      C
ATOM   5618  CG  PRO C 148      94.611  -1.527  -1.697  1.00 30.19      C
ATOM   5619  C   PRO C 148      97.734  -1.327   0.255  1.00 34.28      C
ATOM   5620  O   PRO C 148      98.244  -2.067   1.087  1.00 35.43      C
ATOM   5621  N   GLU C 149      98.441  -0.445  -0.437  1.00 37.73      C
ATOM   5622  CA  GLU C 149      99.873  -0.372  -0.221  1.00 41.17      C
ATOM   5623  CB  GLU C 149     100.532   0.535  -1.266  1.00 39.75      C
ATOM   5624  CG  GLU C 149     102.038   0.662  -1.083  1.00 39.00      C
ATOM   5625  CD  GLU C 149     102.703   1.461  -2.171  1.00 39.73      C
ATOM   5626  OE1 GLU C 149     102.443   2.683  -2.265  1.00 39.67      C
ATOM   5627  OE2 GLU C 149     103.490   0.868  -2.938  1.00 39.04      C
ATOM   5628  C   GLU C 149     100.183   0.120   1.195  1.00 44.52      C
ATOM   5629  O   GLU C 149     100.646  -0.656   2.032  1.00 44.69      C
ATOM   5630  N   GLU C 150      99.914   1.398   1.460  1.00 48.03      C
ATOM   5631  CA  GLU C 150     100.161   1.995   2.774  1.00 51.71      C
ATOM   5632  CB  GLU C 150      99.557   3.407   2.822  1.00 52.60      C
ATOM   5633  CG  GLU C 150     100.095   4.362   1.763  1.00 56.26      C
ATOM   5634  CD  GLU C 150     101.508   4.869   2.052  1.00 57.57      C
ATOM   5635  OE1 GLU C 150     101.735   5.354   3.178  1.00 58.02      C
ATOM   5636  OE2 GLU C 150     102.381   4.803   1.153  1.00 58.12      C
ATOM   5637  C   GLU C 150      99.603   1.136   3.938  1.00 53.38      C
ATOM   5638  O   GLU C 150     100.159   1.112   5.042  1.00 52.61      C
ATOM   5639  N   GLU C 151      98.515   0.420   3.677  1.00 55.17      C
ATOM   5640  CA  GLU C 151      97.891  -0.431   4.681  1.00 58.21      C
ATOM   5641  CB  GLU C 151      96.636  -1.087   4.097  1.00 60.47      C
ATOM   5642  CG  GLU C 151      95.349  -0.835   4.868  1.00 62.11      C
ATOM   5643  CD  GLU C 151      94.154  -1.512   4.222  1.00 63.63      C
ATOM   5644  OE1 GLU C 151      94.025  -1.410   2.978  1.00 64.05      C
ATOM   5645  OE2 GLU C 151      93.347  -2.135   4.955  1.00 63.74      C
ATOM   5646  C   GLU C 151      98.845  -1.519   5.182  1.00 59.56      C
ATOM   5647  O   GLU C 151      99.118  -1.609   6.375  1.00 60.86      C
ATOM   5648  N   ALA C 152      99.345  -2.346   4.269  1.00 60.60      C
ATOM   5649  CA  ALA C 152     100.263  -3.422   4.626  1.00 61.88      C
ATOM   5650  CB  ALA C 152     100.455  -4.356   3.439  1.00 61.89      C
ATOM   5651  C   ALA C 152     101.616  -2.881   5.080  1.00 62.64      C
ATOM   5652  O   ALA C 152     102.398  -3.589   5.699  1.00 62.91      C
ATOM   5653  N   ALA C 153     101.888  -1.622   4.769  1.00 64.35      C
ATOM   5654  CA  ALA C 153     103.146  -1.005   5.144  1.00 66.65      C
ATOM   5655  CB  ALA C 153     103.441   0.166   4.222  1.00 66.57      C
ATOM   5656  C   ALA C 153     103.114  -0.534   6.593  1.00 68.35      C
ATOM   5657  O   ALA C 153     104.159  -0.238   7.177  1.00 67.40      C
ATOM   5658  N   ILE C 154     101.913  -0.463   7.167  1.00 70.84      C
ATOM   5659  CA  ILE C 154     101.753  -0.021   8.549  1.00 73.04      C
ATOM   5660  CB  ILE C 154     100.276   0.333   8.874  1.00 72.44      C
ATOM   5661  CG2 ILE C 154     100.160   0.823  10.308  0.00 73.15      C
ATOM   5662  CG1 ILE C 154      99.768   1.405   7.906  0.00 73.18      C
ATOM   5663  CD1 ILE C 154     100.596   2.681   7.891  0.00 73.32      C
ATOM   5664  C   ILE C 154     102.242  -1.083   9.530  1.00 74.39      C
ATOM   5665  O   ILE C 154     103.164  -0.836  10.314  1.00 75.10      C
ATOM   5666  N   ARG C 155     101.638  -2.267   9.481  1.00 75.33      C
ATOM   5667  CA  ARG C 155     102.035  -3.343  10.386  1.00 77.14      C
```

```
ATOM   5668  CB  ARG C 155     101.354  -4.655   9.970  1.00 77.56      C
ATOM   5669  CG  ARG C 155     101.473  -4.969   8.491  1.00 79.06      C
ATOM   5670  CD  ARG C 155     100.453  -6.012   8.042  1.00 79.84      C
ATOM   5671  NE  ARG C 155     101.032  -7.346   7.880  1.00 82.03      C
ATOM   5672  CZ  ARG C 155     101.458  -8.120   8.876  1.00 83.21      C
ATOM   5673  NH1 ARG C 155     101.376  -7.702  10.130  1.00 83.46      C
ATOM   5674  NH2 ARG C 155     101.967  -9.320   8.617  1.00 83.34      C
ATOM   5675  C   ARG C 155     103.557  -3.521  10.429  1.00 77.49      C
ATOM   5676  O   ARG C 155     104.141  -3.689  11.505  1.00 76.81      C
ATOM   5677  N   ARG C 156     104.185  -3.454   9.256  1.00 78.72      C
ATOM   5678  CA  ARG C 156     105.631  -3.611   9.120  1.00 80.26      C
ATOM   5679  CB  ARG C 156     106.371  -2.543   9.936  1.00 79.66      C
ATOM   5680  CG  ARG C 156     106.197  -1.128   9.442  1.00 78.84      C
ATOM   5681  CD  ARG C 156     106.951  -0.151  10.332  1.00 78.63      C
ATOM   5682  NE  ARG C 156     106.958   1.201   9.777  1.00 79.37      C
ATOM   5683  CZ  ARG C 156     107.560   2.243  10.344  1.00 79.78      C
ATOM   5684  NH1 ARG C 156     108.210   2.098  11.492  1.00 80.21      C
ATOM   5685  NH2 ARG C 156     107.513   3.434   9.763  1.00 79.89      C
ATOM   5686  C   ARG C 156     106.075  -4.997   9.586  1.00 81.59      C
ATOM   5687  O   ARG C 156     106.298  -5.862   8.715  0.00 81.82      C
ATOM   5688  OXT ARG C 156     106.182  -5.207  10.817  1.00 83.28      C
ATOM   5689  CB  LEU D 270      75.377  10.305  15.206  1.00 63.79      D
ATOM   5690  CG  LEU D 270      75.038   9.447  13.983  1.00 64.88      D
ATOM   5691  CD1 LEU D 270      73.550   9.589  13.707  1.00 64.89      D
ATOM   5692  CD2 LEU D 270      75.842   9.894  12.762  1.00 64.87      D
ATOM   5693  C   LEU D 270      77.526   9.458  16.216  1.00 61.89      D
ATOM   5694  O   LEU D 270      78.274   9.273  17.176  1.00 61.69      D
ATOM   5695  N   LEU D 270      75.776  10.456  17.643  1.00 62.12      D
ATOM   5696  CA  LEU D 270      76.015   9.627  16.425  1.00 62.72      D
ATOM   5697  N   LYS D 271      77.975   9.523  14.966  1.00 60.94      D
ATOM   5698  CA  LYS D 271      79.394   9.377  14.666  1.00 59.23      D
ATOM   5699  CB  LYS D 271      79.635   9.177  13.157  1.00 61.06      D
ATOM   5700  CG  LYS D 271      79.243  10.362  12.273  1.00 61.84      D
ATOM   5701  CD  LYS D 271      79.810  10.233  10.859  1.00 62.36      D
ATOM   5702  CE  LYS D 271      81.303  10.589  10.782  1.00 63.95      D
ATOM   5703  NZ  LYS D 271      82.195   9.772  11.664  1.00 62.34      D
ATOM   5704  C   LYS D 271      80.146  10.607  15.114  1.00 56.61      D
ATOM   5705  O   LYS D 271      79.604  11.715  15.119  1.00 56.97      D
ATOM   5706  N   ARG D 272      81.403  10.412  15.483  1.00 53.78      D
ATOM   5707  CA  ARG D 272      82.212  11.531  15.902  1.00 51.25      D
ATOM   5708  CB  ARG D 272      81.625  12.153  17.159  1.00 50.62      D
ATOM   5709  CG  ARG D 272      81.295  13.617  16.977  1.00 50.35      D
ATOM   5710  CD  ARG D 272      82.497  14.465  17.304  1.00 50.29      D
ATOM   5711  NE  ARG D 272      82.835  15.461  16.290  1.00 50.91      D
ATOM   5712  CZ  ARG D 272      82.084  16.507  15.950  1.00 50.34      D
ATOM   5713  NH1 ARG D 272      80.913  16.720  16.528  1.00 50.37      D
ATOM   5714  NH2 ARG D 272      82.528  17.376  15.049  1.00 50.67      D
ATOM   5715  C   ARG D 272      83.652  11.142  16.124  1.00 49.27      D
ATOM   5716  O   ARG D 272      83.995  10.497  17.112  1.00 50.77      D
ATOM   5717  N   ASP D 273      84.498  11.523  15.180  1.00 45.44      D
ATOM   5718  CA  ASP D 273      85.904  11.229  15.310  1.00 40.81      D
ATOM   5719  CB  ASP D 273      86.582  11.281  13.951  1.00 40.44      D
ATOM   5720  CG  ASP D 273      87.998  10.765  13.997  1.00 40.32      D
ATOM   5721  OD1 ASP D 273      88.731  11.138  14.939  1.00 40.48      D
```

```
ATOM   5722  OD2 ASP D 273      88.377   9.991  13.094  1.00 40.70      D
ATOM   5723  C   ASP D 273      86.486  12.295  16.231  1.00 38.02      D
ATOM   5724  O   ASP D 273      87.082  13.269  15.771  1.00 36.97      D
ATOM   5725  N   LEU D 274      86.301  12.096  17.536  1.00 35.35      D
ATOM   5726  CA  LEU D 274      86.783  13.026  18.562  1.00 32.44      D
ATOM   5727  CB  LEU D 274      86.596  12.405  19.957  1.00 32.29      D
ATOM   5728  CG  LEU D 274      85.237  11.729  20.146  1.00 33.44      D
ATOM   5729  CD1 LEU D 274      85.148  10.949  21.454  1.00 33.06      D
ATOM   5730  CD2 LEU D 274      84.185  12.796  20.076  1.00 33.99      D
ATOM   5731  C   LEU D 274      88.250  13.443  18.376  1.00 30.29      D
ATOM   5732  O   LEU D 274      88.589  14.620  18.487  1.00 29.35      D
ATOM   5733  N   ILE D 275      89.119  12.481  18.090  1.00 27.97      D
ATOM   5734  CA  ILE D 275      90.529  12.790  17.919  1.00 26.53      D
ATOM   5735  CB  ILE D 275      91.366  11.487  17.721  1.00 26.41      D
ATOM   5736  CG2 ILE D 275      92.798  11.829  17.316  1.00 25.43      D
ATOM   5737  CG1 ILE D 275      91.390  10.679  19.029  1.00 24.46      D
ATOM   5738  CD1 ILE D 275      92.026  11.404  20.207  1.00 19.75      D
ATOM   5739  C   ILE D 275      90.738  13.764  16.748  1.00 26.48      D
ATOM   5740  O   ILE D 275      91.490  14.743  16.855  1.00 26.90      D
ATOM   5741  N   THR D 276      90.052  13.503  15.642  1.00 24.10      D
ATOM   5742  CA  THR D 276      90.134  14.348  14.469  1.00 22.65      D
ATOM   5743  CB  THR D 276      89.447  13.632  13.273  1.00 21.40      D
ATOM   5744  OG1 THR D 276      90.221  12.483  12.942  1.00 21.35      D
ATOM   5745  CG2 THR D 276      89.321  14.528  12.052  1.00 18.26      D
ATOM   5746  C   THR D 276      89.477  15.711  14.769  1.00 23.50      D
ATOM   5747  O   THR D 276      90.041  16.768  14.462  1.00 22.31      D
ATOM   5748  N   SER D 277      88.305  15.673  15.397  1.00 23.60      D
ATOM   5749  CA  SER D 277      87.582  16.883  15.745  1.00 25.64      D
ATOM   5750  CB  SER D 277      86.156  16.544  16.144  1.00 25.38      D
ATOM   5751  OG  SER D 277      85.440  16.087  15.019  1.00 27.48      D
ATOM   5752  C   SER D 277      88.215  17.739  16.837  1.00 26.65      D
ATOM   5753  O   SER D 277      88.380  18.939  16.657  1.00 29.61      D
ATOM   5754  N   LEU D 278      88.561  17.147  17.970  1.00 25.91      D
ATOM   5755  CA  LEU D 278      89.180  17.922  19.035  1.00 26.38      D
ATOM   5756  CB  LEU D 278      89.564  17.027  20.218  1.00 26.10      D
ATOM   5757  CG  LEU D 278      88.426  16.811  21.194  1.00 24.98      D
ATOM   5758  CD1 LEU D 278      88.017  18.153  21.792  1.00 26.21      D
ATOM   5759  CD2 LEU D 278      87.257  16.190  20.458  1.00 28.73      D
ATOM   5760  C   LEU D 278      90.426  18.621  18.530  1.00 26.46      D
ATOM   5761  O   LEU D 278      91.038  18.189  17.549  1.00 27.90      D
ATOM   5762  N   PRO D 279      90.803  19.733  19.177  1.00 26.62      D
ATOM   5763  CD  PRO D 279      89.970  20.521  20.096  1.00 26.92      D
ATOM   5764  CA  PRO D 279      91.994  20.496  18.799  1.00 27.49      D
ATOM   5765  CB  PRO D 279      91.940  21.686  19.739  1.00 26.12      D
ATOM   5766  CG  PRO D 279      90.495  21.922  19.861  1.00 25.59      D
ATOM   5767  C   PRO D 279      93.212  19.620  19.047  1.00 29.22      D
ATOM   5768  O   PRO D 279      93.221  18.827  19.991  1.00 30.55      D
ATOM   5769  N   PHE D 280      94.234  19.775  18.210  1.00 29.38      D
ATOM   5770  CA  PHE D 280      95.452  18.980  18.303  1.00 29.08      D
ATOM   5771  CB  PHE D 280      96.567  19.668  17.518  1.00 30.38      D
ATOM   5772  CG  PHE D 280      97.839  18.871  17.438  1.00 33.85      D
ATOM   5773  CD1 PHE D 280      97.849  17.585  16.890  1.00 35.64      D
ATOM   5774  CD2 PHE D 280      99.038  19.415  17.886  1.00 34.62      D
ATOM   5775  CE1 PHE D 280      99.045  16.852  16.789  1.00 36.28      D
```

```
ATOM   5776  CE2 PHE D 280     100.237  18.696  17.790  1.00 35.86      D
ATOM   5777  CZ  PHE D 280     100.242  17.410  17.239  1.00 36.27      D
ATOM   5778  C   PHE D 280      95.883  18.747  19.746  1.00 28.87      D
ATOM   5779  O   PHE D 280      96.100  17.611  20.167  1.00 28.22      D
ATOM   5780  N   GLU D 281      95.977  19.824  20.513  1.00 29.70      D
ATOM   5781  CA  GLU D 281      96.394  19.735  21.906  1.00 30.73      D
ATOM   5782  CB  GLU D 281      96.367  21.124  22.544  1.00 30.74      D
ATOM   5783  CG  GLU D 281      96.958  22.225  21.686  1.00 35.82      D
ATOM   5784  CD  GLU D 281      96.181  22.455  20.365  1.00 39.11      D
ATOM   5785  OE1 GLU D 281      94.927  22.371  20.364  1.00 37.33      D
ATOM   5786  OE2 GLU D 281      96.838  22.734  19.329  1.00 41.78      D
ATOM   5787  C   GLU D 281      95.508  18.767  22.707  1.00 30.47      D
ATOM   5788  O   GLU D 281      95.998  17.800  23.291  1.00 29.60      D
ATOM   5789  N   ILE D 282      94.200  19.006  22.731  1.00 30.62      D
ATOM   5790  CA  ILE D 282      93.326  18.115  23.495  1.00 30.51      D
ATOM   5791  CB  ILE D 282      91.826  18.479  23.367  1.00 28.68      D
ATOM   5792  CG2 ILE D 282      90.973  17.454  24.096  1.00 25.40      D
ATOM   5793  CG1 ILE D 282      91.559  19.841  24.002  1.00 28.37      D
ATOM   5794  CD1 ILE D 282      92.338  20.960  23.374  1.00 29.50      D
ATOM   5795  C   ILE D 282      93.506  16.667  23.085  1.00 30.93      D
ATOM   5796  O   ILE D 282      93.569  15.798  23.939  1.00 32.03      D
ATOM   5797  N   SER D 283      93.597  16.403  21.786  1.00 33.38      D
ATOM   5798  CA  SER D 283      93.773  15.037  21.315  1.00 33.57      D
ATOM   5799  CB  SER D 283      93.729  14.991  19.793  1.00 33.09      D
ATOM   5800  OG  SER D 283      92.440  14.625  19.343  1.00 33.69      D
ATOM   5801  C   SER D 283      95.060  14.383  21.806  1.00 34.43      D
ATOM   5802  O   SER D 283      95.102  13.171  21.996  1.00 35.71      D
ATOM   5803  N   LEU D 284      96.121  15.158  21.996  1.00 33.67      D
ATOM   5804  CA  LEU D 284      97.345  14.541  22.479  1.00 33.99      D
ATOM   5805  CB  LEU D 284      98.511  15.514  22.412  1.00 34.78      D
ATOM   5806  CG  LEU D 284      98.908  15.828  20.966  1.00 37.92      D
ATOM   5807  CD1 LEU D 284      99.965  16.921  20.972  1.00 38.44      D
ATOM   5808  CD2 LEU D 284      99.424  14.571  20.264  1.00 35.81      D
ATOM   5809  C   LEU D 284      97.105  14.089  23.908  1.00 34.14      D
ATOM   5810  O   LEU D 284      97.469  12.972  24.268  1.00 35.96      D
ATOM   5811  N   LYS D 285      96.470  14.944  24.710  1.00 32.83      D
ATOM   5812  CA  LYS D 285      96.180  14.598  26.094  1.00 31.02      D
ATOM   5813  CB  LYS D 285      95.192  15.590  26.711  1.00 32.29      D
ATOM   5814  CG  LYS D 285      95.694  17.027  26.672  1.00 34.86      D
ATOM   5815  CD  LYS D 285      94.977  17.944  27.659  1.00 38.81      D
ATOM   5816  CE  LYS D 285      95.626  17.931  29.043  1.00 41.32      D
ATOM   5817  NZ  LYS D 285      95.083  19.055  29.866  1.00 43.73      D
ATOM   5818  C   LYS D 285      95.603  13.194  26.129  1.00 28.79      D
ATOM   5819  O   LYS D 285      96.124  12.305  26.823  1.00 29.62      D
ATOM   5820  N   ILE D 286      94.538  12.991  25.360  1.00 25.19      D
ATOM   5821  CA  ILE D 286      93.898  11.681  25.281  1.00 24.05      D
ATOM   5822  CB  ILE D 286      92.834  11.660  24.148  1.00 22.82      D
ATOM   5823  CG2 ILE D 286      92.176  10.291  24.060  1.00 21.24      D
ATOM   5824  CG1 ILE D 286      91.800  12.757  24.414  1.00 23.94      D
ATOM   5825  CD1 ILE D 286      90.731  12.886  23.321  1.00 23.24      D
ATOM   5826  C   ILE D 286      94.950  10.583  25.036  1.00 23.79      D
ATOM   5827  O   ILE D 286      94.970   9.573  25.738  1.00 22.04      D
ATOM   5828  N   PHE D 287      95.825  10.788  24.051  1.00 21.07      D
ATOM   5829  CA  PHE D 287      96.844   9.790  23.746  1.00 21.11      D
```

```
ATOM   5830  CB  PHE D 287      97.596  10.147  22.469  1.00 20.53      D
ATOM   5831  CG  PHE D 287      96.842   9.818  21.221  1.00 20.94      D
ATOM   5832  CD1 PHE D 287      96.528   8.495  20.915  1.00 18.61      D
ATOM   5833  CD2 PHE D 287      96.445  10.831  20.340  1.00 20.85      D
ATOM   5834  CE1 PHE D 287      95.835   8.184  19.754  1.00 17.26      D
ATOM   5835  CE2 PHE D 287      95.752  10.525  19.177  1.00 18.21      D
ATOM   5836  CZ  PHE D 287      95.444   9.204  18.876  1.00 16.07      D
ATOM   5837  C   PHE D 287      97.849   9.539  24.859  1.00 21.96      D
ATOM   5838  O   PHE D 287      98.314   8.418  25.035  1.00 20.26      D
ATOM   5839  N   ASN D 288      98.182  10.592  25.593  1.00 23.06      D
ATOM   5840  CA  ASN D 288      99.128  10.494  26.677  1.00 25.24      D
ATOM   5841  CB  ASN D 288      99.598  11.892  27.089  1.00 25.50      D
ATOM   5842  CG  ASN D 288     100.691  12.432  26.166  1.00 27.45      D
ATOM   5843  OD1 ASN D 288     101.539  11.660  25.680  1.00 29.10      D
ATOM   5844  ND2 ASN D 288     100.696  13.750  25.936  1.00 25.61      D
ATOM   5845  C   ASN D 288      98.585   9.695  27.883  1.00 28.89      D
ATOM   5846  O   ASN D 288      99.331   9.376  28.815  1.00 28.16      D
ATOM   5847  N   TYR D 289      97.289   9.368  27.846  1.00 30.81      D
ATOM   5848  CA  TYR D 289      96.633   8.560  28.879  1.00 33.41      D
ATOM   5849  CB  TYR D 289      95.210   9.038  29.193  1.00 35.09      D
ATOM   5850  CG  TYR D 289      95.100  10.237  30.098  1.00 38.19      D
ATOM   5851  CD1 TYR D 289      95.713  10.256  31.343  1.00 37.23      D
ATOM   5852  CE1 TYR D 289      95.585  11.353  32.182  1.00 37.83      D
ATOM   5853  CD2 TYR D 289      94.353  11.348  29.713  1.00 38.71      D
ATOM   5854  CE2 TYR D 289      94.219  12.447  30.543  1.00 39.19      D
ATOM   5855  CZ  TYR D 289      94.838  12.449  31.778  1.00 38.07      D
ATOM   5856  OH  TYR D 289      94.716  13.558  32.596  1.00 37.65      D
ATOM   5857  C   TYR D 289      96.496   7.129  28.375  1.00 34.42      D
ATOM   5858  O   TYR D 289      95.852   6.288  29.016  1.00 34.85      D
ATOM   5859  N   LEU D 290      97.076   6.857  27.215  1.00 34.95      D
ATOM   5860  CA  LEU D 290      96.980   5.530  26.632  1.00 36.71      D
ATOM   5861  CB  LEU D 290      96.488   5.621  25.189  1.00 37.91      D
ATOM   5862  CG  LEU D 290      95.004   5.925  24.991  1.00 38.82      D
ATOM   5863  CD1 LEU D 290      94.740   6.136  23.516  1.00 39.93      D
ATOM   5864  CD2 LEU D 290      94.159   4.764  25.535  1.00 37.72      D
ATOM   5865  C   LEU D 290      98.302   4.802  26.664  1.00 37.19      D
ATOM   5866  O   LEU D 290      99.354   5.419  26.628  1.00 37.91      D
ATOM   5867  N   GLN D 291      98.256   3.482  26.744  1.00 38.53      D
ATOM   5868  CA  GLN D 291      99.493   2.736  26.771  1.00 39.34      D
ATOM   5869  CB  GLN D 291      99.251   1.308  27.236  1.00 40.51      D
ATOM   5870  CG  GLN D 291      98.786   1.213  28.657  1.00 43.34      D
ATOM   5871  CD  GLN D 291      98.666  -0.215  29.102  1.00 46.99      D
ATOM   5872  OE1 GLN D 291      99.662  -0.945  29.172  1.00 50.86      D
ATOM   5873  NE2 GLN D 291      97.444  -0.638  29.398  1.00 49.26      D
ATOM   5874  C   GLN D 291     100.090   2.749  25.374  1.00 38.68      D
ATOM   5875  O   GLN D 291      99.393   2.990  24.383  1.00 39.01      D
ATOM   5876  N   PHE D 292     101.386   2.482  25.308  1.00 35.62      D
ATOM   5877  CA  PHE D 292     102.096   2.492  24.059  1.00 32.95      D
ATOM   5878  CB  PHE D 292     103.583   2.209  24.335  1.00 32.02      D
ATOM   5879  CG  PHE D 292     104.010   0.795  24.109  1.00 29.67      D
ATOM   5880  CD1 PHE D 292     104.290   0.349  22.829  1.00 30.05      D
ATOM   5881  CD2 PHE D 292     104.221  -0.064  25.176  1.00 29.27      D
ATOM   5882  CE1 PHE D 292     104.788  -0.932  22.613  1.00 30.66      D
ATOM   5883  CE2 PHE D 292     104.719  -1.348  24.972  1.00 29.01      D
```

```
ATOM   5884  CZ  PHE D 292     105.004  -1.781  23.686  1.00 29.86      D
ATOM   5885  C   PHE D 292     101.477   1.552  23.035  1.00 32.44      D
ATOM   5886  O   PHE D 292     101.384   1.894  21.852  1.00 33.62      D
ATOM   5887  N   GLU D 293     101.018   0.389  23.481  1.00 31.32      D
ATOM   5888  CA  GLU D 293     100.396  -0.551  22.560  1.00 29.89      D
ATOM   5889  CB  GLU D 293      99.974  -1.819  23.296  1.00 29.10      D
ATOM   5890  CG  GLU D 293     101.135  -2.712  23.586  1.00 30.44      D
ATOM   5891  CD  GLU D 293     101.534  -2.717  25.053  1.00 31.93      D
ATOM   5892  OE1 GLU D 293     101.473  -1.647  25.722  1.00 28.98      D
ATOM   5893  OE2 GLU D 293     101.924  -3.815  25.518  1.00 32.42      D
ATOM   5894  C   GLU D 293      99.187   0.044  21.864  1.00 28.52      D
ATOM   5895  O   GLU D 293      98.978  -0.193  20.679  1.00 26.63      D
ATOM   5896  N   ASP D 294      98.391   0.802  22.615  1.00 29.50      D
ATOM   5897  CA  ASP D 294      97.193   1.431  22.081  1.00 30.32      D
ATOM   5898  CB  ASP D 294      96.330   2.030  23.210  1.00 32.63      D
ATOM   5899  CG  ASP D 294      95.768   0.968  24.183  1.00 36.82      D
ATOM   5900  OD1 ASP D 294      95.503  -0.192  23.772  1.00 39.44      D
ATOM   5901  OD2 ASP D 294      95.563   1.309  25.369  1.00 38.44      D
ATOM   5902  C   ASP D 294      97.585   2.542  21.103  1.00 29.40      D
ATOM   5903  O   ASP D 294      96.796   2.930  20.245  1.00 27.84      D
ATOM   5904  N   ILE D 295      98.805   3.050  21.237  1.00 28.17      D
ATOM   5905  CA  ILE D 295      99.266   4.114  20.362  1.00 28.34      D
ATOM   5906  CB  ILE D 295     100.510   4.784  20.917  1.00 28.05      D
ATOM   5907  CG2 ILE D 295     100.845   5.998  20.077  1.00 25.51      D
ATOM   5908  CG1 ILE D 295     100.294   5.145  22.392  1.00 30.16      D
ATOM   5909  CD1 ILE D 295      99.338   6.283  22.658  1.00 31.34      D
ATOM   5910  C   ILE D 295      99.605   3.549  18.990  1.00 28.98      D
ATOM   5911  O   ILE D 295      99.310   4.151  17.956  1.00 28.75      D
ATOM   5912  N   ILE D 296     100.227   2.381  18.996  1.00 29.17      D
ATOM   5913  CA  ILE D 296     100.612   1.715  17.768  1.00 30.36      D
ATOM   5914  CB  ILE D 296     101.521   0.491  18.085  1.00 30.31      D
ATOM   5915  CG2 ILE D 296     101.236  -0.660  17.148  1.00 28.53      D
ATOM   5916  CG1 ILE D 296     102.987   0.911  17.989  1.00 31.04      D
ATOM   5917  CD1 ILE D 296     103.353   2.115  18.829  1.00 32.07      D
ATOM   5918  C   ILE D 296      99.379   1.308  16.965  1.00 30.74      D
ATOM   5919  O   ILE D 296      99.376   1.398  15.741  1.00 30.48      D
ATOM   5920  N   ASN D 297      98.330   0.865  17.642  1.00 31.12      D
ATOM   5921  CA  ASN D 297      97.121   0.506  16.924  1.00 33.08      D
ATOM   5922  CB  ASN D 297      96.096  -0.099  17.865  1.00 33.38      D
ATOM   5923  CG  ASN D 297      96.393  -1.537  18.171  1.00 37.25      D
ATOM   5924  OD1 ASN D 297      95.953  -2.067  19.194  1.00 37.85      D
ATOM   5925  ND2 ASN D 297      97.143  -2.196  17.270  1.00 37.30      D
ATOM   5926  C   ASN D 297      96.548   1.767  16.316  1.00 33.81      D
ATOM   5927  O   ASN D 297      96.220   1.817  15.123  1.00 34.30      D
ATOM   5928  N   SER D 298      96.435   2.780  17.168  1.00 32.14      D
ATOM   5929  CA  SER D 298      95.912   4.079  16.792  1.00 30.45      D
ATOM   5930  CB  SER D 298      96.100   5.073  17.939  1.00 29.96      D
ATOM   5931  OG  SER D 298      95.395   4.648  19.087  1.00 27.42      D
ATOM   5932  C   SER D 298      96.656   4.566  15.583  1.00 30.58      D
ATOM   5933  O   SER D 298      96.103   5.255  14.731  1.00 32.34      D
ATOM   5934  N   LEU D 299      97.930   4.216  15.514  1.00 29.49      D
ATOM   5935  CA  LEU D 299      98.738   4.628  14.387  1.00 28.00      D
ATOM   5936  CB  LEU D 299     100.164   4.131  14.570  1.00 28.12      D
ATOM   5937  CG  LEU D 299     101.291   5.098  14.240  1.00 28.83      D
```

```
ATOM   5938  CD1 LEU D 299     101.105   6.442  14.938  1.00 28.49      D
ATOM   5939  CD2 LEU D 299     102.595   4.455  14.703  1.00 30.72      D
ATOM   5940  C   LEU D 299      98.147   4.063  13.108  1.00 27.04      D
ATOM   5941  O   LEU D 299      98.382   4.608  12.045  1.00 28.76      D
ATOM   5942  N   GLY D 300      97.356   2.996  13.212  1.00 25.60      D
ATOM   5943  CA  GLY D 300      96.783   2.387  12.018  1.00 25.16      D
ATOM   5944  C   GLY D 300      95.268   2.423  11.857  1.00 25.49      D
ATOM   5945  O   GLY D 300      94.665   1.528  11.258  1.00 24.96      D
ATOM   5946  N   VAL D 301      94.661   3.476  12.381  1.00 26.14      D
ATOM   5947  CA  VAL D 301      93.223   3.677  12.335  1.00 25.65      D
ATOM   5948  CB  VAL D 301      92.783   4.425  13.635  1.00 25.13      D
ATOM   5949  CG1 VAL D 301      91.377   4.975  13.523  1.00 23.49      D
ATOM   5950  CG2 VAL D 301      92.881   3.470  14.818  1.00 25.09      D
ATOM   5951  C   VAL D 301      92.853   4.482  11.085  1.00 26.83      D
ATOM   5952  O   VAL D 301      91.895   4.160  10.386  1.00 29.06      D
ATOM   5953  N   SER D 302      93.624   5.517  10.781  1.00 27.15      D
ATOM   5954  CA  SER D 302      93.321   6.327   9.611  1.00 27.14      D
ATOM   5955  CB  SER D 302      92.021   7.096   9.832  1.00 26.96      D
ATOM   5956  OG  SER D 302      92.186   8.048  10.876  1.00 28.29      D
ATOM   5957  C   SER D 302      94.442   7.308   9.329  1.00 26.93      D
ATOM   5958  O   SER D 302      95.174   7.696  10.239  1.00 27.64      D
ATOM   5959  N   GLN D 303      94.558   7.720   8.067  1.00 26.82      D
ATOM   5960  CA  GLN D 303      95.596   8.658   7.661  1.00 25.04      D
ATOM   5961  CB  GLN D 303      95.362   9.166   6.244  1.00 23.83      D
ATOM   5962  CG  GLN D 303      95.865   8.261   5.154  1.00 29.99      D
ATOM   5963  CD  GLN D 303      97.398   8.160   5.090  1.00 32.84      D
ATOM   5964  OE1 GLN D 303      97.942   7.457   4.239  1.00 34.49      D
ATOM   5965  NE2 GLN D 303      98.091   8.863   5.986  1.00 36.06      D
ATOM   5966  C   GLN D 303      95.653   9.852   8.587  1.00 23.97      D
ATOM   5967  O   GLN D 303      96.743  10.343   8.901  1.00 22.53      D
ATOM   5968  N   ASN D 304      94.490  10.322   9.034  1.00 22.85      D
ATOM   5969  CA  ASN D 304      94.479  11.487   9.908  1.00 24.54      D
ATOM   5970  CB  ASN D 304      93.082  12.042  10.095  1.00 25.34      D
ATOM   5971  CG  ASN D 304      93.105  13.358  10.814  1.00 28.24      D
ATOM   5972  OD1 ASN D 304      92.215  13.657  11.613  1.00 30.04      D
ATOM   5973  ND2 ASN D 304      94.143  14.163  10.544  1.00 29.46      D
ATOM   5974  C   ASN D 304      95.058  11.172  11.270  1.00 25.25      D
ATOM   5975  O   ASN D 304      95.876  11.928  11.820  1.00 24.93      D
ATOM   5976  N   TRP D 305      94.609  10.063  11.835  1.00 25.15      D
ATOM   5977  CA  TRP D 305      95.139   9.658  13.118  1.00 25.51      D
ATOM   5978  CB  TRP D 305      94.447   8.373  13.587  1.00 25.43      D
ATOM   5979  CG  TRP D 305      93.138   8.630  14.311  1.00 26.00      D
ATOM   5980  CD2 TRP D 305      92.614   7.880  15.410  1.00 26.49      D
ATOM   5981  CE2 TRP D 305      91.351   8.425  15.730  1.00 24.97      D
ATOM   5982  CE3 TRP D 305      93.090   6.796  16.157  1.00 27.62      D
ATOM   5983  CD1 TRP D 305      92.199   9.581  14.015  1.00 25.09      D
ATOM   5984  NE1 TRP D 305      91.122   9.461  14.864  1.00 24.10      D
ATOM   5985  CZ2 TRP D 305      90.559   7.918  16.764  1.00 23.76      D
ATOM   5986  CZ3 TRP D 305      92.299   6.297  17.183  1.00 25.00      D
ATOM   5987  CH2 TRP D 305      91.053   6.859  17.474  1.00 24.03      D
ATOM   5988  C   TRP D 305      96.656   9.477  12.935  1.00 24.69      D
ATOM   5989  O   TRP D 305      97.445   9.992  13.734  1.00 25.68      D
ATOM   5990  N   ASN D 306      97.054   8.786  11.863  1.00 22.23      D
ATOM   5991  CA  ASN D 306      98.471   8.583  11.555  1.00 21.36      D
```

```
ATOM   5992  CB  ASN D 306      98.669   7.946  10.182  1.00 19.88      D
ATOM   5993  CG  ASN D 306     100.134   7.572   9.920  1.00 20.62      D
ATOM   5994  OD1 ASN D 306     100.608   6.526  10.394  1.00 21.63      D
ATOM   5995  ND2 ASN D 306     100.860   8.427   9.176  1.00 16.92      D
ATOM   5996  C   ASN D 306      99.203   9.913  11.517  1.00 21.93      D
ATOM   5997  O   ASN D 306     100.356  10.009  11.912  1.00 21.70      D
ATOM   5998  N   LYS D 307      98.533  10.930  11.000  1.00 22.01      D
ATOM   5999  CA  LYS D 307      99.134  12.235  10.907  1.00 23.12      D
ATOM   6000  CB  LYS D 307      98.270  13.136  10.027  1.00 24.42      D
ATOM   6001  CG  LYS D 307      98.897  14.469   9.657  1.00 25.07      D
ATOM   6002  CD  LYS D 307      97.803  15.504   9.446  1.00 29.41      D
ATOM   6003  CE  LYS D 307      98.290  16.723   8.650  1.00 31.20      D
ATOM   6004  NZ  LYS D 307      98.710  16.351   7.251  1.00 30.25      D
ATOM   6005  C   LYS D 307      99.298  12.868  12.284  1.00 24.28      D
ATOM   6006  O   LYS D 307     100.387  13.292  12.654  1.00 26.10      D
ATOM   6007  N   ILE D 308      98.214  12.902  13.047  1.00 23.74      D
ATOM   6008  CA  ILE D 308      98.217  13.520  14.359  1.00 25.31      D
ATOM   6009  CB  ILE D 308      96.843  13.350  15.042  1.00 27.23      D
ATOM   6010  CG2 ILE D 308      96.899  13.810  16.475  1.00 27.28      D
ATOM   6011  CG1 ILE D 308      95.794  14.187  14.294  1.00 28.70      D
ATOM   6012  CD1 ILE D 308      94.383  14.048  14.808  1.00 26.95      D
ATOM   6013  C   ILE D 308      99.298  13.018  15.292  1.00 25.96      D
ATOM   6014  O   ILE D 308     100.079  13.797  15.838  1.00 24.81      D
ATOM   6015  N   ILE D 309      99.353  11.710  15.464  1.00 26.12      D
ATOM   6016  CA  ILE D 309     100.314  11.115  16.359  1.00 25.75      D
ATOM   6017  CB  ILE D 309      99.990   9.603  16.538  1.00 25.30      D
ATOM   6018  CG2 ILE D 309     100.995   8.937  17.437  1.00 24.21      D
ATOM   6019  CG1 ILE D 309      98.617   9.437  17.181  1.00 21.52      D
ATOM   6020  CD1 ILE D 309      98.160   8.023  17.261  1.00 23.28      D
ATOM   6021  C   ILE D 309     101.755  11.313  15.906  1.00 26.74      D
ATOM   6022  O   ILE D 309     102.626  11.586  16.729  1.00 27.84      D
ATOM   6023  N   ARG D 310     102.026  11.177  14.610  1.00 28.38      D
ATOM   6024  CA  ARG D 310     103.401  11.350  14.098  1.00 29.18      D
ATOM   6025  CB  ARG D 310     103.513  10.811  12.663  1.00 28.52      D
ATOM   6026  CG  ARG D 310     103.531   9.277  12.560  1.00 30.67      D
ATOM   6027  CD  ARG D 310     103.052   8.787  11.186  1.00 34.25      D
ATOM   6028  NE  ARG D 310     104.098   8.252  10.323  1.00 36.16      D
ATOM   6029  CZ  ARG D 310     105.097   8.969   9.827  1.00 38.55      D
ATOM   6030  NH1 ARG D 310     105.200  10.259  10.095  1.00 42.20      D
ATOM   6031  NH2 ARG D 310     106.009   8.391   9.069  1.00 41.89      D
ATOM   6032  C   ARG D 310     103.838  12.811  14.139  1.00 28.88      D
ATOM   6033  O   ARG D 310     104.996  13.133  13.873  1.00 28.32      D
ATOM   6034  N   LYS D 311     102.900  13.681  14.496  1.00 29.76      D
ATOM   6035  CA  LYS D 311     103.172  15.104  14.570  1.00 32.11      D
ATOM   6036  CB  LYS D 311     101.894  15.868  14.227  1.00 32.03      D
ATOM   6037  CG  LYS D 311     102.061  17.362  14.098  1.00 36.15      D
ATOM   6038  CD  LYS D 311     100.731  18.049  13.814  1.00 39.43      D
ATOM   6039  CE  LYS D 311     100.895  19.580  13.814  1.00 42.31      D
ATOM   6040  NZ  LYS D 311     100.575  20.231  15.122  1.00 42.00      D
ATOM   6041  C   LYS D 311     103.728  15.564  15.934  1.00 32.85      D
ATOM   6042  O   LYS D 311     104.467  16.545  15.992  1.00 32.33      D
ATOM   6043  N   SER D 312     103.395  14.855  17.017  1.00 33.76      D
ATOM   6044  CA  SER D 312     103.857  15.223  18.365  1.00 33.60      D
ATOM   6045  CB  SER D 312     102.835  14.787  19.421  1.00 35.34      D
```

```
ATOM   6046  OG  SER D 312     103.198  15.271  20.712  1.00 39.47      D
ATOM   6047  C   SER D 312     105.222  14.667  18.781  1.00 31.68      D
ATOM   6048  O   SER D 312     105.456  13.468  18.728  1.00 32.40      D
ATOM   6049  N   THR D 313     106.125  15.543  19.198  1.00 30.17      D
ATOM   6050  CA  THR D 313     107.429  15.095  19.651  1.00 29.28      D
ATOM   6051  CB  THR D 313     108.502  16.214  19.480  1.00 30.08      D
ATOM   6052  OG1 THR D 313     109.122  16.072  18.199  1.00 31.16      D
ATOM   6053  CG2 THR D 313     109.580  16.132  20.558  1.00 30.05      D
ATOM   6054  C   THR D 313     107.270  14.701  21.128  1.00 27.77      D
ATOM   6055  O   THR D 313     107.658  13.603  21.538  1.00 26.51      D
ATOM   6056  N   SER D 314     106.666  15.599  21.901  1.00 26.12      D
ATOM   6057  CA  SER D 314     106.420  15.370  23.311  1.00 26.42      D
ATOM   6058  CB  SER D 314     105.499  16.454  23.886  1.00 25.86      D
ATOM   6059  OG  SER D 314     104.133  16.191  23.589  1.00 25.20      D
ATOM   6060  C   SER D 314     105.755  14.011  23.534  1.00 26.86      D
ATOM   6061  O   SER D 314     106.064  13.314  24.486  1.00 27.19      D
ATOM   6062  N   LEU D 315     104.830  13.633  22.668  1.00 26.78      D
ATOM   6063  CA  LEU D 315     104.169  12.368  22.851  1.00 26.12      D
ATOM   6064  CB  LEU D 315     103.148  12.167  21.741  1.00 25.84      D
ATOM   6065  CG  LEU D 315     102.212  10.960  21.711  1.00 26.39      D
ATOM   6066  CD1 LEU D 315     101.094  11.269  20.721  1.00 27.77      D
ATOM   6067  CD2 LEU D 315     102.933   9.691  21.303  1.00 24.47      D
ATOM   6068  C   LEU D 315     105.186  11.229  22.899  1.00 26.05      D
ATOM   6069  O   LEU D 315     105.108  10.373  23.780  1.00 27.85      D
ATOM   6070  N   TRP D 316     106.165  11.224  21.998  1.00 24.50      D
ATOM   6071  CA  TRP D 316     107.141  10.138  22.011  1.00 25.89      D
ATOM   6072  CB  TRP D 316     107.751   9.952  20.607  1.00 24.16      D
ATOM   6073  CG  TRP D 316     106.708   9.452  19.635  1.00 21.27      D
ATOM   6074  CD2 TRP D 316     106.177   8.123  19.565  1.00 18.61      D
ATOM   6075  CE2 TRP D 316     105.107   8.146  18.646  1.00 18.90      D
ATOM   6076  CE3 TRP D 316     106.498   6.917  20.193  1.00 20.19      D
ATOM   6077  CD1 TRP D 316     105.959  10.206  18.767  1.00 20.28      D
ATOM   6078  NE1 TRP D 316     104.994   9.428  18.177  1.00 19.42      D
ATOM   6079  CZ2 TRP D 316     104.351   7.007  18.344  1.00 19.58      D
ATOM   6080  CZ3 TRP D 316     105.741   5.778  19.892  1.00 21.16      D
ATOM   6081  CH2 TRP D 316     104.682   5.835  18.975  1.00 20.34      D
ATOM   6082  C   TRP D 316     108.216  10.292  23.091  1.00 27.23      D
ATOM   6083  O   TRP D 316     108.854   9.311  23.519  1.00 27.64      D
ATOM   6084  N   LYS D 317     108.374  11.525  23.556  1.00 27.58      D
ATOM   6085  CA  LYS D 317     109.332  11.847  24.602  1.00 27.23      D
ATOM   6086  CB  LYS D 317     109.463  13.360  24.759  1.00 29.14      D
ATOM   6087  CG  LYS D 317     110.589  13.760  25.682  1.00 32.80      D
ATOM   6088  CD  LYS D 317     110.743  15.264  25.749  1.00 35.26      D
ATOM   6089  CE  LYS D 317     111.774  15.652  26.805  1.00 37.31      D
ATOM   6090  NZ  LYS D 317     111.793  17.120  27.068  1.00 37.03      D
ATOM   6091  C   LYS D 317     108.822  11.275  25.910  1.00 25.94      D
ATOM   6092  O   LYS D 317     109.570  10.685  26.689  1.00 25.94      D
ATOM   6093  N   LYS D 318     107.533  11.473  26.142  1.00 23.54      D
ATOM   6094  CA  LYS D 318     106.921  10.980  27.345  1.00 21.52      D
ATOM   6095  CB  LYS D 318     105.457  11.403  27.426  1.00 19.84      D
ATOM   6096  CG  LYS D 318     105.276  12.802  27.949  1.00 15.81      D
ATOM   6097  CD  LYS D 318     103.822  13.127  28.039  1.00 17.16      D
ATOM   6098  CE  LYS D 318     103.592  14.588  28.439  1.00 19.94      D
ATOM   6099  NZ  LYS D 318     104.446  15.524  27.676  1.00 22.18      D
```

```
ATOM   6100  C   LYS D 318     107.026   9.474  27.389  1.00 21.47      D
ATOM   6101  O   LYS D 318     107.353   8.890  28.423  1.00 22.72      D
ATOM   6102  N   LEU D 319     106.754   8.825  26.271  1.00 20.41      D
ATOM   6103  CA  LEU D 319     106.834   7.373  26.259  1.00 19.54      D
ATOM   6104  CB  LEU D 319     106.427   6.839  24.894  1.00 17.41      D
ATOM   6105  CG  LEU D 319     104.933   6.610  24.750  1.00 14.60      D
ATOM   6106  CD1 LEU D 319     104.590   6.417  23.307  1.00 15.84      D
ATOM   6107  CD2 LEU D 319     104.520   5.398  25.581  1.00 13.04      D
ATOM   6108  C   LEU D 319     108.232   6.901  26.605  1.00 19.33      D
ATOM   6109  O   LEU D 319     108.395   6.014  27.441  1.00 18.41      D
ATOM   6110  N   LEU D 320     109.239   7.493  25.961  1.00 20.82      D
ATOM   6111  CA  LEU D 320     110.624   7.099  26.217  1.00 21.24      D
ATOM   6112  CB  LEU D 320     111.589   7.926  25.344  1.00 17.94      D
ATOM   6113  CG  LEU D 320     111.710   7.492  23.869  1.00 18.89      D
ATOM   6114  CD1 LEU D 320     112.467   8.533  23.030  1.00 16.82      D
ATOM   6115  CD2 LEU D 320     112.402   6.158  23.797  1.00 15.44      D
ATOM   6116  C   LEU D 320     110.965   7.259  27.701  1.00 22.18      D
ATOM   6117  O   LEU D 320     111.574   6.383  28.310  1.00 23.23      D
ATOM   6118  N   ILE D 321     110.545   8.375  28.281  1.00 22.59      D
ATOM   6119  CA  ILE D 321     110.824   8.661  29.676  1.00 22.13      D
ATOM   6120  CB  ILE D 321     110.462  10.125  30.007  1.00 21.71      D
ATOM   6121  CG2 ILE D 321     110.406  10.336  31.509  1.00 20.64      D
ATOM   6122  CG1 ILE D 321     111.471  11.053  29.324  1.00 20.39      D
ATOM   6123  CD1 ILE D 321     111.312  12.527  29.639  1.00 17.62      D
ATOM   6124  C   ILE D 321     110.112   7.729  30.641  1.00 21.87      D
ATOM   6125  O   ILE D 321     110.726   7.204  31.551  1.00 23.61      D
ATOM   6126  N   SER D 322     108.819   7.526  30.449  1.00 22.79      D
ATOM   6127  CA  SER D 322     108.082   6.663  31.345  1.00 23.92      D
ATOM   6128  CB  SER D 322     106.610   6.624  30.943  1.00 24.36      D
ATOM   6129  OG  SER D 322     106.464   6.398  29.554  1.00 28.99      D
ATOM   6130  C   SER D 322     108.668   5.256  31.377  1.00 25.68      D
ATOM   6131  O   SER D 322     108.780   4.660  32.440  1.00 27.76      D
ATOM   6132  N   GLU D 323     109.041   4.718  30.222  1.00 24.70      D
ATOM   6133  CA  GLU D 323     109.625   3.389  30.188  1.00 23.55      D
ATOM   6134  CB  GLU D 323     109.581   2.835  28.775  1.00 24.33      D
ATOM   6135  CG  GLU D 323     108.228   2.303  28.385  1.00 25.11      D
ATOM   6136  CD  GLU D 323     107.953   0.951  29.008  1.00 26.37      D
ATOM   6137  OE1 GLU D 323     108.775   0.024  28.805  1.00 26.30      D
ATOM   6138  OE2 GLU D 323     106.920   0.809  29.695  1.00 27.36      D
ATOM   6139  C   GLU D 323     111.059   3.448  30.678  1.00 23.31      D
ATOM   6140  O   GLU D 323     111.773   2.443  30.684  1.00 23.15      D
ATOM   6141  N   ASN D 324     111.467   4.644  31.091  1.00 22.23      D
ATOM   6142  CA  ASN D 324     112.812   4.891  31.592  1.00 22.59      D
ATOM   6143  CB  ASN D 324     113.038   4.090  32.877  1.00 22.90      D
ATOM   6144  CG  ASN D 324     111.864   4.200  33.858  1.00 26.71      D
ATOM   6145  OD1 ASN D 324     111.346   5.294  34.109  1.00 25.11      D
ATOM   6146  ND2 ASN D 324     111.450   3.056  34.430  1.00 28.34      D
ATOM   6147  C   ASN D 324     113.911   4.565  30.560  1.00 23.12      D
ATOM   6148  O   ASN D 324     114.971   4.031  30.914  1.00 23.08      D
ATOM   6149  N   PHE D 325     113.667   4.881  29.285  1.00 22.49      D
ATOM   6150  CA  PHE D 325     114.673   4.613  28.246  1.00 22.20      D
ATOM   6151  CB  PHE D 325     114.005   4.332  26.882  1.00 18.54      D
ATOM   6152  CG  PHE D 325     113.296   2.991  26.806  1.00 18.28      D
ATOM   6153  CD1 PHE D 325     112.080   2.864  26.117  1.00 17.36      D
```

```
ATOM   6154  CD2 PHE D 325     113.828   1.860  27.425  1.00 17.01      D
ATOM   6155  CE1 PHE D 325     111.404   1.631  26.053  1.00 15.65      D
ATOM   6156  CE2 PHE D 325     113.165   0.617  27.369  1.00 16.41      D
ATOM   6157  CZ  PHE D 325     111.942   0.508  26.677  1.00 16.67      D
ATOM   6158  C   PHE D 325     115.640   5.798  28.136  1.00 21.95      D
ATOM   6159  O   PHE D 325     116.735   5.686  27.578  1.00 21.44      D
ATOM   6160  N   VAL D 326     115.240   6.925  28.707  1.00 21.18      D
ATOM   6161  CA  VAL D 326     116.059   8.113  28.642  1.00 21.85      D
ATOM   6162  CB  VAL D 326     115.922   8.765  27.238  1.00 21.90      D
ATOM   6163  CG1 VAL D 326     114.455   9.085  26.972  1.00 22.16      D
ATOM   6164  CG2 VAL D 326     116.772  10.016  27.133  1.00 19.90      D
ATOM   6165  C   VAL D 326     115.619   9.084  29.725  1.00 22.99      D
ATOM   6166  O   VAL D 326     114.453   9.105  30.121  1.00 23.26      D
ATOM   6167  N   SER D 327     116.571   9.869  30.215  1.00 26.57      D
ATOM   6168  CA  SER D 327     116.308  10.853  31.257  1.00 30.18      D
ATOM   6169  CB  SER D 327     117.552  11.111  32.099  1.00 28.88      D
ATOM   6170  OG  SER D 327     117.794  10.061  33.008  1.00 34.20      D
ATOM   6171  C   SER D 327     115.914  12.167  30.648  1.00 32.93      D
ATOM   6172  O   SER D 327     116.304  12.488  29.533  1.00 33.50      D
ATOM   6173  N   PRO D 328     115.141  12.958  31.384  1.00 36.30      D
ATOM   6174  CD  PRO D 328     114.483  12.591  32.644  1.00 38.28      D
ATOM   6175  CA  PRO D 328     114.693  14.269  30.923  1.00 38.59      D
ATOM   6176  CB  PRO D 328     113.988  14.834  32.140  1.00 38.19      D
ATOM   6177  CG  PRO D 328     113.360  13.609  32.728  1.00 39.16      D
ATOM   6178  C   PRO D 328     115.900  15.110  30.526  1.00 40.86      D
ATOM   6179  O   PRO D 328     115.886  15.787  29.496  1.00 42.18      D
ATOM   6180  N   LYS D 329     116.955  15.053  31.332  1.00 41.28      D
ATOM   6181  CA  LYS D 329     118.143  15.826  31.027  1.00 42.86      D
ATOM   6182  CB  LYS D 329     118.861  16.228  32.327  1.00 46.62      D
ATOM   6183  CG  LYS D 329     118.066  17.272  33.169  1.00 49.10      D
ATOM   6184  CD  LYS D 329     118.615  17.445  34.594  1.00 50.67      D
ATOM   6185  CE  LYS D 329     120.077  17.887  34.606  1.00 51.76      D
ATOM   6186  NZ  LYS D 329     120.645  17.988  35.993  1.00 51.50      D
ATOM   6187  C   LYS D 329     119.078  15.102  30.073  1.00 42.35      D
ATOM   6188  O   LYS D 329     120.060  15.671  29.609  1.00 43.19      D
ATOM   6189  N   GLY D 330     118.766  13.850  29.765  1.00 41.86      D
ATOM   6190  CA  GLY D 330     119.597  13.107  28.837  1.00 40.87      D
ATOM   6191  C   GLY D 330     118.961  13.089  27.456  1.00 42.32      D
ATOM   6192  O   GLY D 330     119.470  12.461  26.528  1.00 41.14      D
ATOM   6193  N   PHE D 331     117.849  13.798  27.304  1.00 44.29      D
ATOM   6194  CA  PHE D 331     117.148  13.809  26.026  1.00 46.40      D
ATOM   6195  CB  PHE D 331     115.887  14.660  26.119  1.00 47.33      D
ATOM   6196  CG  PHE D 331     114.896  14.396  25.016  1.00 49.12      D
ATOM   6197  CD1 PHE D 331     114.198  13.188  24.958  1.00 48.42      D
ATOM   6198  CD2 PHE D 331     114.658  15.359  24.033  1.00 49.78      D
ATOM   6199  CE1 PHE D 331     113.273  12.942  23.939  1.00 48.28      D
ATOM   6200  CE2 PHE D 331     113.735  15.128  23.008  1.00 49.07      D
ATOM   6201  CZ  PHE D 331     113.042  13.917  22.958  1.00 49.05      D
ATOM   6202  C   PHE D 331     117.983  14.276  24.846  1.00 46.95      D
ATOM   6203  O   PHE D 331     118.017  13.613  23.815  1.00 48.73      D
ATOM   6204  N   ASN D 332     118.651  15.414  24.997  1.00 47.11      D
ATOM   6205  CA  ASN D 332     119.477  15.972  23.932  1.00 46.02      D
ATOM   6206  CB  ASN D 332     120.255  17.161  24.463  1.00 47.82      D
ATOM   6207  CG  ASN D 332     119.497  18.440  24.335  1.00 49.50      D
```

```
ATOM   6208  OD1 ASN D 332     118.322  18.519  24.692  1.00 50.47      D
ATOM   6209  ND2 ASN D 332     120.165  19.468  23.815  1.00 52.34      D
ATOM   6210  C   ASN D 332     120.451  14.972  23.336  1.00 45.93      D
ATOM   6211  O   ASN D 332     120.420  14.681  22.140  1.00 45.54      D
ATOM   6212  N   SER D 333     121.326  14.443  24.175  1.00 46.43      D
ATOM   6213  CA  SER D 333     122.308  13.487  23.702  1.00 45.98      D
ATOM   6214  CB  SER D 333     123.043  12.863  24.885  1.00 46.48      D
ATOM   6215  OG  SER D 333     123.853  11.783  24.454  1.00 49.00      D
ATOM   6216  C   SER D 333     121.659  12.392  22.851  1.00 44.33      D
ATOM   6217  O   SER D 333     122.129  12.099  21.751  1.00 44.40      D
ATOM   6218  N   LEU D 334     120.577  11.795  23.344  1.00 42.68      D
ATOM   6219  CA  LEU D 334     119.912  10.728  22.591  1.00 41.52      D
ATOM   6220  CB  LEU D 334     118.777  10.098  23.407  1.00 39.72      D
ATOM   6221  CG  LEU D 334     117.873   9.152  22.604  1.00 38.51      D
ATOM   6222  CD1 LEU D 334     118.687   7.997  22.053  1.00 37.25      D
ATOM   6223  CD2 LEU D 334     116.746   8.651  23.475  1.00 37.57      D
ATOM   6224  C   LEU D 334     119.352  11.228  21.268  1.00 39.88      D
ATOM   6225  O   LEU D 334     119.439  10.553  20.242  1.00 37.95      D
ATOM   6226  N   ASN D 335     118.758  12.410  21.304  1.00 39.39      D
ATOM   6227  CA  ASN D 335     118.202  12.973  20.096  1.00 39.71      D
ATOM   6228  CB  ASN D 335     117.463  14.263  20.399  1.00 40.92      D
ATOM   6229  CG  ASN D 335     116.080  14.255  19.829  1.00 42.75      D
ATOM   6230  OD1 ASN D 335     115.879  13.877  18.676  1.00 43.99      D
ATOM   6231  ND2 ASN D 335     115.108  14.669  20.630  1.00 44.96      D
ATOM   6232  C   ASN D 335     119.299  13.229  19.066  1.00 38.88      D
ATOM   6233  O   ASN D 335     119.209  12.772  17.926  1.00 39.28      D
ATOM   6234  N   LEU D 336     120.341  13.945  19.469  1.00 36.54      D
ATOM   6235  CA  LEU D 336     121.426  14.216  18.555  1.00 35.78      D
ATOM   6236  CB  LEU D 336     122.488  15.081  19.230  1.00 35.28      D
ATOM   6237  CG  LEU D 336     123.704  15.571  18.421  1.00 35.06      D
ATOM   6238  CD1 LEU D 336     124.755  14.482  18.364  1.00 33.88      D
ATOM   6239  CD2 LEU D 336     123.284  16.002  17.027  1.00 33.93      D
ATOM   6240  C   LEU D 336     122.021  12.905  18.034  1.00 36.03      D
ATOM   6241  O   LEU D 336     122.542  12.857  16.920  1.00 37.69      D
ATOM   6242  N   LYS D 337     121.919  11.833  18.812  1.00 36.19      D
ATOM   6243  CA  LYS D 337     122.439  10.529  18.378  1.00 37.20      D
ATOM   6244  CB  LYS D 337     122.452   9.533  19.547  1.00 38.40      D
ATOM   6245  CG  LYS D 337     123.706   9.512  20.409  1.00 40.10      D
ATOM   6246  CD  LYS D 337     124.743   8.543  19.848  1.00 41.01      D
ATOM   6247  CE  LYS D 337     125.896   8.283  20.827  1.00 41.41      D
ATOM   6248  NZ  LYS D 337     125.504   7.528  22.071  1.00 40.33      D
ATOM   6249  C   LYS D 337     121.576   9.939  17.257  1.00 37.31      D
ATOM   6250  O   LYS D 337     122.081   9.279  16.344  1.00 37.48      D
ATOM   6251  N   LEU D 338     120.268  10.164  17.347  1.00 36.91      D
ATOM   6252  CA  LEU D 338     119.332   9.654  16.351  1.00 36.87      D
ATOM   6253  CB  LEU D 338     117.893   9.797  16.863  1.00 35.09      D
ATOM   6254  CG  LEU D 338     117.529   8.902  18.052  1.00 33.33      D
ATOM   6255  CD1 LEU D 338     116.175   9.300  18.621  1.00 31.89      D
ATOM   6256  CD2 LEU D 338     117.533   7.450  17.600  1.00 31.70      D
ATOM   6257  C   LEU D 338     119.513  10.412  15.044  1.00 37.22      D
ATOM   6258  O   LEU D 338     119.418   9.841  13.968  1.00 36.68      D
ATOM   6259  N   SER D 339     119.791  11.703  15.161  1.00 37.23      D
ATOM   6260  CA  SER D 339     120.000  12.537  14.006  1.00 35.92      D
ATOM   6261  CB  SER D 339     120.390  13.933  14.426  1.00 34.24      D
```

```
ATOM   6262  OG  SER D 339     120.457  14.756  13.283  1.00 37.68      D
ATOM   6263  C   SER D 339     121.094  11.973  13.124  1.00 36.83      D
ATOM   6264  O   SER D 339     120.978  12.005  11.908  1.00 36.94      D
ATOM   6265  N   GLN D 340     122.161  11.467  13.735  1.00 36.98      D
ATOM   6266  CA  GLN D 340     123.266  10.895  12.975  1.00 37.54      D
ATOM   6267  CB  GLN D 340     124.443  10.581  13.883  1.00 38.76      D
ATOM   6268  CG  GLN D 340     124.489  11.408  15.144  1.00 42.76      D
ATOM   6269  CD  GLN D 340     125.519  12.491  15.095  1.00 43.21      D
ATOM   6270  OE1 GLN D 340     125.816  13.113  16.105  1.00 43.96      D
ATOM   6271  NE2 GLN D 340     126.077  12.727  13.917  1.00 47.75      D
ATOM   6272  C   GLN D 340     122.786   9.592  12.376  1.00 38.02      D
ATOM   6273  O   GLN D 340     123.099   9.254  11.235  1.00 36.84      D
ATOM   6274  N   LYS D 341     122.023   8.857  13.172  1.00 38.91      D
ATOM   6275  CA  LYS D 341     121.503   7.564  12.759  1.00 40.04      D
ATOM   6276  CB  LYS D 341     120.908   6.842  13.979  1.00 41.15      D
ATOM   6277  CG  LYS D 341     120.440   5.417  13.722  1.00 43.83      D
ATOM   6278  CD  LYS D 341     121.542   4.580  13.081  1.00 46.84      D
ATOM   6279  CE  LYS D 341     121.018   3.233  12.559  1.00 48.14      D
ATOM   6280  NZ  LYS D 341     122.101   2.428  11.901  1.00 48.02      D
ATOM   6281  C   LYS D 341     120.463   7.656  11.641  1.00 40.03      D
ATOM   6282  O   LYS D 341     120.548   6.935  10.647  1.00 40.71      D
ATOM   6283  N   TYR D 342     119.494   8.551  11.804  1.00 39.52      D
ATOM   6284  CA  TYR D 342     118.413   8.726  10.840  1.00 39.22      D
ATOM   6285  CB  TYR D 342     117.084   8.349  11.504  1.00 40.25      D
ATOM   6286  CG  TYR D 342     117.093   6.975  12.120  1.00 41.96      D
ATOM   6287  CD1 TYR D 342     117.151   5.839  11.322  1.00 44.58      D
ATOM   6288  CE1 TYR D 342     117.195   4.559  11.887  1.00 46.16      D
ATOM   6289  CD2 TYR D 342     117.076   6.805  13.501  1.00 43.49      D
ATOM   6290  CE2 TYR D 342     117.119   5.530  14.078  1.00 44.33      D
ATOM   6291  CZ  TYR D 342     117.180   4.412  13.263  1.00 45.41      D
ATOM   6292  OH  TYR D 342     117.244   3.145  13.796  1.00 44.64      D
ATOM   6293  C   TYR D 342     118.315  10.155  10.287  1.00 38.30      D
ATOM   6294  O   TYR D 342     117.437  10.926  10.687  1.00 38.68      D
ATOM   6295  N   PRO D 343     119.207  10.522   9.354  1.00 36.69      D
ATOM   6296  CD  PRO D 343     120.303   9.690   8.831  1.00 33.93      D
ATOM   6297  CA  PRO D 343     119.222  11.859   8.744  1.00 35.64      D
ATOM   6298  CB  PRO D 343     120.322  11.747   7.701  1.00 33.94      D
ATOM   6299  CG  PRO D 343     121.227  10.708   8.264  1.00 33.00      D
ATOM   6300  C   PRO D 343     117.897  12.243   8.100  1.00 36.66      D
ATOM   6301  O   PRO D 343     117.387  13.353   8.298  1.00 36.68      D
ATOM   6302  N   LYS D 344     117.345  11.306   7.333  1.00 37.98      D
ATOM   6303  CA  LYS D 344     116.097  11.521   6.600  1.00 38.87      D
ATOM   6304  CB  LYS D 344     116.021  10.554   5.402  1.00 40.52      D
ATOM   6305  CG  LYS D 344     116.552   9.140   5.658  1.00 43.94      D
ATOM   6306  CD  LYS D 344     115.598   8.274   6.494  1.00 44.39      D
ATOM   6307  CE  LYS D 344     116.370   7.166   7.227  1.00 43.37      D
ATOM   6308  NZ  LYS D 344     117.439   7.751   8.094  1.00 37.93      D
ATOM   6309  C   LYS D 344     114.791  11.471   7.396  1.00 37.24      D
ATOM   6310  O   LYS D 344     113.779  12.011   6.947  1.00 38.60      D
ATOM   6311  N   LEU D 345     114.808  10.851   8.572  1.00 34.93      D
ATOM   6312  CA  LEU D 345     113.597  10.766   9.382  1.00 32.64      D
ATOM   6313  CB  LEU D 345     113.670   9.573  10.329  1.00 31.24      D
ATOM   6314  CG  LEU D 345     113.726   8.216   9.628  1.00 29.39      D
ATOM   6315  CD1 LEU D 345     113.660   7.118  10.667  1.00 30.86      D
```

```
ATOM   6316  CD2 LEU D 345     112.560   8.084   8.666  1.00 30.92      D
ATOM   6317  C   LEU D 345     113.376  12.033  10.176  1.00 31.59      D
ATOM   6318  O   LEU D 345     114.318  12.780  10.422  1.00 32.92      D
ATOM   6319  N   SER D 346     112.130  12.298  10.557  1.00 30.59      D
ATOM   6320  CA  SER D 346     111.836  13.500  11.338  1.00 29.97      D
ATOM   6321  CB  SER D 346     110.377  13.931  11.158  1.00 29.48      D
ATOM   6322  OG  SER D 346     109.498  12.856  11.422  1.00 30.59      D
ATOM   6323  C   SER D 346     112.101  13.212  12.800  1.00 29.74      D
ATOM   6324  O   SER D 346     112.387  12.069  13.184  1.00 28.91      D
ATOM   6325  N   GLN D 347     111.992  14.233  13.634  1.00 28.38      D
ATOM   6326  CA  GLN D 347     112.255  13.991  15.036  1.00 28.40      D
ATOM   6327  CB  GLN D 347     112.237  15.291  15.818  1.00 29.66      D
ATOM   6328  CG  GLN D 347     112.819  15.144  17.190  1.00 32.02      D
ATOM   6329  CD  GLN D 347     112.905  16.474  17.879  1.00 35.29      D
ATOM   6330  OE1 GLN D 347     111.889  17.161  18.035  1.00 38.15      D
ATOM   6331  NE2 GLN D 347     114.111  16.861  18.292  1.00 33.64      D
ATOM   6332  C   GLN D 347     111.277  13.007  15.663  1.00 26.76      D
ATOM   6333  O   GLN D 347     111.694  12.085  16.357  1.00 26.57      D
ATOM   6334  N   GLN D 348     109.984  13.203  15.427  1.00 25.38      D
ATOM   6335  CA  GLN D 348     108.996  12.306  16.001  1.00 24.96      D
ATOM   6336  CB  GLN D 348     107.581  12.739  15.657  1.00 24.21      D
ATOM   6337  CG  GLN D 348     107.267  14.152  16.034  1.00 24.28      D
ATOM   6338  CD  GLN D 348     107.648  15.126  14.947  1.00 23.84      D
ATOM   6339  OE1 GLN D 348     108.598  14.899  14.211  1.00 24.03      D
ATOM   6340  NE2 GLN D 348     106.908  16.224  14.845  1.00 24.64      D
ATOM   6341  C   GLN D 348     109.209  10.896  15.483  1.00 26.54      D
ATOM   6342  O   GLN D 348     109.118   9.921  16.233  1.00 27.22      D
ATOM   6343  N   ASP D 349     109.499  10.791  14.193  1.00 26.70      D
ATOM   6344  CA  ASP D 349     109.718   9.500  13.588  1.00 26.16      D
ATOM   6345  CB  ASP D 349     109.918   9.666  12.086  1.00 30.05      D
ATOM   6346  CG  ASP D 349     108.666   9.338  11.295  1.00 33.76      D
ATOM   6347  OD1 ASP D 349     107.598   9.889  11.612  1.00 35.36      D
ATOM   6348  OD2 ASP D 349     108.754   8.521  10.354  1.00 37.16      D
ATOM   6349  C   ASP D 349     110.900   8.775  14.220  1.00 25.17      D
ATOM   6350  O   ASP D 349     110.815   7.578  14.508  1.00 25.67      D
ATOM   6351  N   ARG D 350     111.999   9.491  14.430  1.00 23.55      D
ATOM   6352  CA  ARG D 350     113.194   8.906  15.047  1.00 23.54      D
ATOM   6353  CB  ARG D 350     114.265   9.981  15.252  1.00 25.20      D
ATOM   6354  CG  ARG D 350     114.885  10.512  13.994  1.00 25.82      D
ATOM   6355  CD  ARG D 350     115.595  11.837  14.220  1.00 25.92      D
ATOM   6356  NE  ARG D 350     116.255  12.230  12.977  1.00 28.94      D
ATOM   6357  CZ  ARG D 350     116.707  13.448  12.698  1.00 29.47      D
ATOM   6358  NH1 ARG D 350     116.590  14.440  13.568  1.00 32.83      D
ATOM   6359  NH2 ARG D 350     117.281  13.673  11.534  1.00 31.17      D
ATOM   6360  C   ARG D 350     112.831   8.343  16.416  1.00 23.18      D
ATOM   6361  O   ARG D 350     112.968   7.148  16.679  1.00 22.24      D
ATOM   6362  N   LEU D 351     112.376   9.242  17.282  1.00 21.94      D
ATOM   6363  CA  LEU D 351     111.991   8.890  18.627  1.00 20.55      D
ATOM   6364  CB  LEU D 351     111.307  10.082  19.297  1.00 18.30      D
ATOM   6365  CG  LEU D 351     112.227  11.278  19.543  1.00 15.70      D
ATOM   6366  CD1 LEU D 351     111.401  12.443  19.998  1.00 14.97      D
ATOM   6367  CD2 LEU D 351     113.315  10.927  20.561  1.00 12.36      D
ATOM   6368  C   LEU D 351     111.081   7.671  18.627  1.00 20.79      D
ATOM   6369  O   LEU D 351     111.175   6.824  19.508  1.00 21.85      D
```

```
ATOM   6370  N   ARG D 352     110.211   7.569  17.631  1.00 21.27      D
ATOM   6371  CA  ARG D 352     109.333   6.421  17.566  1.00 22.32      D
ATOM   6372  CB  ARG D 352     108.251   6.616  16.517  1.00 23.50      D
ATOM   6373  CG  ARG D 352     107.278   5.440  16.398  1.00 25.41      D
ATOM   6374  CD  ARG D 352     106.075   5.874  15.568  1.00 26.94      D
ATOM   6375  NE  ARG D 352     106.491   6.312  14.248  1.00 27.67      D
ATOM   6376  CZ  ARG D 352     106.345   5.590  13.151  1.00 27.98      D
ATOM   6377  NH1 ARG D 352     105.772   4.384  13.223  1.00 28.77      D
ATOM   6378  NH2 ARG D 352     106.801   6.071  11.997  1.00 28.35      D
ATOM   6379  C   ARG D 352     110.132   5.156  17.257  1.00 22.65      D
ATOM   6380  O   ARG D 352     109.852   4.088  17.809  1.00 22.75      D
ATOM   6381  N   LEU D 353     111.129   5.236  16.389  1.00 23.22      D
ATOM   6382  CA  LEU D 353     111.877   4.014  16.139  1.00 25.64      D
ATOM   6383  CB  LEU D 353     112.853   4.180  14.974  1.00 27.60      D
ATOM   6384  CG  LEU D 353     112.211   4.675  13.687  1.00 31.53      D
ATOM   6385  CD1 LEU D 353     113.257   4.543  12.590  1.00 34.73      D
ATOM   6386  CD2 LEU D 353     110.948   3.847  13.321  1.00 34.02      D
ATOM   6387  C   LEU D 353     112.640   3.650  17.408  1.00 24.34      D
ATOM   6388  O   LEU D 353     112.766   2.477  17.748  1.00 24.26      D
ATOM   6389  N   SER D 354     113.135   4.654  18.124  1.00 24.48      D
ATOM   6390  CA  SER D 354     113.888   4.379  19.339  1.00 24.64      D
ATOM   6391  CB  SER D 354     114.399   5.670  19.953  1.00 24.29      D
ATOM   6392  OG  SER D 354     115.774   5.509  20.223  1.00 27.22      D
ATOM   6393  C   SER D 354     113.045   3.623  20.345  1.00 23.77      D
ATOM   6394  O   SER D 354     113.439   2.566  20.828  1.00 22.40      D
ATOM   6395  N   PHE D 355     111.879   4.169  20.646  1.00 23.57      D
ATOM   6396  CA  PHE D 355     110.979   3.533  21.573  1.00 25.63      D
ATOM   6397  CB  PHE D 355     109.660   4.283  21.596  1.00 26.61      D
ATOM   6398  CG  PHE D 355     108.725   3.795  22.636  1.00 27.78      D
ATOM   6399  CD1 PHE D 355     109.055   3.919  23.978  1.00 29.88      D
ATOM   6400  CD2 PHE D 355     107.526   3.189  22.286  1.00 29.67      D
ATOM   6401  CE1 PHE D 355     108.205   3.443  24.972  1.00 29.34      D
ATOM   6402  CE2 PHE D 355     106.664   2.707  23.269  1.00 30.25      D
ATOM   6403  CZ  PHE D 355     107.011   2.836  24.614  1.00 29.64      D
ATOM   6404  C   PHE D 355     110.731   2.089  21.156  1.00 26.53      D
ATOM   6405  O   PHE D 355     110.970   1.156  21.920  1.00 26.93      D
ATOM   6406  N   LEU D 356     110.257   1.904  19.931  1.00 27.97      D
ATOM   6407  CA  LEU D 356     109.975   0.557  19.441  1.00 29.40      D
ATOM   6408  CB  LEU D 356     109.502   0.601  17.990  1.00 29.41      D
ATOM   6409  CG  LEU D 356     108.233   1.408  17.701  1.00 30.81      D
ATOM   6410  CD1 LEU D 356     108.091   1.510  16.193  1.00 30.03      D
ATOM   6411  CD2 LEU D 356     107.001   0.766  18.334  1.00 27.79      D
ATOM   6412  C   LEU D 356     111.164  -0.387  19.557  1.00 29.19      D
ATOM   6413  O   LEU D 356     111.011  -1.540  19.954  1.00 29.03      D
ATOM   6414  N   GLU D 357     112.348   0.106  19.223  1.00 29.15      D
ATOM   6415  CA  GLU D 357     113.525  -0.723  19.296  1.00 30.63      D
ATOM   6416  CB  GLU D 357     114.677  -0.053  18.560  1.00 32.16      D
ATOM   6417  CG  GLU D 357     115.697  -1.025  18.007  1.00 37.30      D
ATOM   6418  CD  GLU D 357     117.086  -0.418  17.930  1.00 40.82      D
ATOM   6419  OE1 GLU D 357     117.248   0.639  17.262  1.00 41.37      D
ATOM   6420  OE2 GLU D 357     118.017  -1.000  18.548  1.00 41.48      D
ATOM   6421  C   GLU D 357     113.946  -1.025  20.741  1.00 32.26      D
ATOM   6422  O   GLU D 357     114.599  -2.041  21.016  1.00 31.90      D
ATOM   6423  N   ASN D 358     113.571  -0.148  21.665  1.00 29.36      D
```

```
ATOM   6424  CA  ASN D 358     113.939  -0.341  23.046  1.00 27.42      D
ATOM   6425  CB  ASN D 358     114.060   1.000  23.750  1.00 27.90      D
ATOM   6426  CG  ASN D 358     115.443   1.598  23.610  1.00 28.81      D
ATOM   6427  OD1 ASN D 358     115.621   2.656  23.006  1.00 29.58      D
ATOM   6428  ND2 ASN D 358     116.439   0.916  24.171  1.00 29.80      D
ATOM   6429  C   ASN D 358     112.996  -1.248  23.793  1.00 27.49      D
ATOM   6430  O   ASN D 358     113.404  -1.974  24.700  1.00 27.75      D
ATOM   6431  N   ILE D 359     111.732  -1.217  23.408  1.00 27.57      D
ATOM   6432  CA  ILE D 359     110.757  -2.076  24.046  1.00 28.89      D
ATOM   6433  CB  ILE D 359     109.361  -1.821  23.510  1.00 29.72      D
ATOM   6434  CG2 ILE D 359     108.342  -2.575  24.322  1.00 28.76      D
ATOM   6435  CG1 ILE D 359     109.058  -0.336  23.581  1.00 32.82      D
ATOM   6436  CD1 ILE D 359     108.196   0.120  22.444  1.00 36.53      D
ATOM   6437  C   ILE D 359     111.161  -3.466  23.629  1.00 28.09      D
ATOM   6438  O   ILE D 359     111.164  -4.389  24.425  1.00 27.60      D
ATOM   6439  N   PHE D 360     111.518  -3.592  22.361  1.00 29.39      D
ATOM   6440  CA  PHE D 360     111.926  -4.864  21.810  1.00 30.15      D
ATOM   6441  CB  PHE D 360     112.415  -4.654  20.372  1.00 32.47      D
ATOM   6442  CG  PHE D 360     112.998  -5.885  19.738  1.00 33.66      D
ATOM   6443  CD1 PHE D 360     112.236  -7.045  19.600  1.00 34.21      D
ATOM   6444  CD2 PHE D 360     114.327  -5.898  19.326  1.00 34.66      D
ATOM   6445  CE1 PHE D 360     112.790  -8.201  19.071  1.00 34.86      D
ATOM   6446  CE2 PHE D 360     114.894  -7.044  18.796  1.00 36.23      D
ATOM   6447  CZ  PHE D 360     114.124  -8.202  18.670  1.00 35.77      D
ATOM   6448  C   PHE D 360     113.015  -5.503  22.654  1.00 29.32      D
ATOM   6449  O   PHE D 360     112.879  -6.641  23.092  1.00 29.82      D
ATOM   6450  N   ILE D 361     114.093  -4.762  22.880  1.00 28.24      D
ATOM   6451  CA  ILE D 361     115.222  -5.254  23.660  1.00 26.57      D
ATOM   6452  CB  ILE D 361     116.376  -4.219  23.597  1.00 26.56      D
ATOM   6453  CG2 ILE D 361     117.540  -4.638  24.502  1.00 24.26      D
ATOM   6454  CG1 ILE D 361     116.855  -4.117  22.140  1.00 25.22      D
ATOM   6455  CD1 ILE D 361     117.841  -3.000  21.868  1.00 25.88      D
ATOM   6456  C   ILE D 361     114.834  -5.578  25.111  1.00 25.14      D
ATOM   6457  O   ILE D 361     115.238  -6.610  25.656  1.00 24.17      D
ATOM   6458  N   LEU D 362     114.027  -4.712  25.718  1.00 22.80      D
ATOM   6459  CA  LEU D 362     113.591  -4.915  27.098  1.00 23.19      D
ATOM   6460  CB  LEU D 362     112.801  -3.700  27.576  1.00 20.92      D
ATOM   6461  CG  LEU D 362     112.565  -3.604  29.077  1.00 20.66      D
ATOM   6462  CD1 LEU D 362     113.860  -3.753  29.867  1.00 18.78      D
ATOM   6463  CD2 LEU D 362     111.917  -2.273  29.338  1.00 20.71      D
ATOM   6464  C   LEU D 362     112.773  -6.196  27.330  1.00 23.63      D
ATOM   6465  O   LEU D 362     112.997  -6.915  28.311  1.00 23.67      D
ATOM   6466  N   LYS D 363     111.824  -6.453  26.434  1.00 23.53      D
ATOM   6467  CA  LYS D 363     110.986  -7.639  26.477  1.00 24.42      D
ATOM   6468  CB  LYS D 363     110.156  -7.743  25.191  1.00 26.43      D
ATOM   6469  CG  LYS D 363     108.730  -7.209  25.270  1.00 30.86      D
ATOM   6470  CD  LYS D 363     108.669  -5.840  25.929  1.00 33.41      D
ATOM   6471  CE  LYS D 363     107.226  -5.421  26.252  1.00 35.72      D
ATOM   6472  NZ  LYS D 363     107.204  -4.294  27.264  1.00 35.50      D
ATOM   6473  C   LYS D 363     111.901  -8.859  26.573  1.00 25.36      D
ATOM   6474  O   LYS D 363     111.629  -9.802  27.311  1.00 25.60      D
ATOM   6475  N   ASN D 364     112.988  -8.829  25.809  1.00 25.23      D
ATOM   6476  CA  ASN D 364     113.935  -9.927  25.799  1.00 25.39      D
ATOM   6477  CB  ASN D 364     114.980  -9.737  24.712  1.00 25.02      D
```

```
ATOM   6478  CG  ASN D 364     114.436  -9.985  23.348  1.00 26.12      D
ATOM   6479  OD1 ASN D 364     115.038  -9.589  22.348  1.00 25.32      D
ATOM   6480  ND2 ASN D 364     113.286 -10.662  23.283  1.00 27.95      D
ATOM   6481  C   ASN D 364     114.640 -10.030  27.118  1.00 26.63      D
ATOM   6482  O   ASN D 364     114.785 -11.120  27.665  1.00 28.76      D
ATOM   6483  N   TRP D 365     115.101  -8.901  27.635  1.00 26.04      D
ATOM   6484  CA  TRP D 365     115.794  -8.937  28.906  1.00 25.62      D
ATOM   6485  CB  TRP D 365     116.211  -7.535  29.357  1.00 23.36      D
ATOM   6486  CG  TRP D 365     117.514  -7.035  28.789  1.00 19.48      D
ATOM   6487  CD2 TRP D 365     118.801  -7.069  29.427  1.00 16.99      D
ATOM   6488  CE2 TRP D 365     119.706  -6.410  28.572  1.00 15.60      D
ATOM   6489  CE3 TRP D 365     119.275  -7.589  30.640  1.00 15.17      D
ATOM   6490  CD1 TRP D 365     117.691  -6.387  27.613  1.00 17.39      D
ATOM   6491  NE1 TRP D 365     119.001  -6.003  27.473  1.00 14.98      D
ATOM   6492  CZ2 TRP D 365     121.072  -6.249  28.892  1.00 15.36      D
ATOM   6493  CZ3 TRP D 365     120.628  -7.428  30.956  1.00 13.84      D
ATOM   6494  CH2 TRP D 365     121.509  -6.762  30.081  1.00 10.82      D
ATOM   6495  C   TRP D 365     114.868  -9.538  29.947  1.00 26.26      D
ATOM   6496  O   TRP D 365     115.267 -10.422  30.693  1.00 28.48      D
ATOM   6497  N   TYR D 366     113.621  -9.084  29.956  1.00 24.80      D
ATOM   6498  CA  TYR D 366     112.641  -9.530  30.934  1.00 23.32      D
ATOM   6499  CB  TYR D 366     111.480  -8.553  30.947  1.00 17.63      D
ATOM   6500  CG  TYR D 366     111.793  -7.211  31.597  1.00 16.02      D
ATOM   6501  CD1 TYR D 366     113.058  -6.914  32.118  1.00 14.32      D
ATOM   6502  CE1 TYR D 366     113.304  -5.681  32.726  1.00 11.48      D
ATOM   6503  CD2 TYR D 366     110.808  -6.243  31.712  1.00 13.79      D
ATOM   6504  CE2 TYR D 366     111.054  -5.033  32.320  1.00 11.61      D
ATOM   6505  CZ  TYR D 366     112.283  -4.760  32.812  1.00 11.97      D
ATOM   6506  OH  TYR D 366     112.475  -3.532  33.364  1.00 15.79      D
ATOM   6507  C   TYR D 366     112.112 -10.939  30.762  1.00 25.30      D
ATOM   6508  O   TYR D 366     111.620 -11.548  31.715  1.00 25.60      D
ATOM   6509  N   ASN D 367     112.227 -11.441  29.538  1.00 27.79      D
ATOM   6510  CA  ASN D 367     111.757 -12.770  29.160  1.00 28.52      D
ATOM   6511  CB  ASN D 367     111.596 -12.837  27.642  1.00 29.23      D
ATOM   6512  CG  ASN D 367     111.047 -14.162  27.168  1.00 29.51      D
ATOM   6513  OD1 ASN D 367     111.045 -15.165  27.907  1.00 29.16      D
ATOM   6514  ND2 ASN D 367     110.588 -14.183  25.915  1.00 28.51      D
ATOM   6515  C   ASN D 367     112.706 -13.872  29.617  1.00 28.04      D
ATOM   6516  O   ASN D 367     113.779 -14.076  29.042  1.00 28.99      D
ATOM   6517  N   PRO D 368     112.306 -14.606  30.659  1.00 27.46      D
ATOM   6518  CD  PRO D 368     111.038 -14.427  31.394  1.00 27.49      D
ATOM   6519  CA  PRO D 368     113.094 -15.701  31.228  1.00 26.35      D
ATOM   6520  CB  PRO D 368     112.174 -16.249  32.313  1.00 26.40      D
ATOM   6521  CG  PRO D 368     111.350 -15.041  32.703  1.00 26.24      D
ATOM   6522  C   PRO D 368     113.470 -16.766  30.207  1.00 25.90      D
ATOM   6523  O   PRO D 368     114.556 -17.338  30.270  1.00 23.69      D
ATOM   6524  N   LYS D 369     112.570 -17.027  29.264  1.00 26.98      D
ATOM   6525  CA  LYS D 369     112.815 -18.051  28.249  1.00 27.69      D
ATOM   6526  CB  LYS D 369     111.483 -18.478  27.605  1.00 27.37      D
ATOM   6527  CG  LYS D 369     111.523 -19.857  26.933  1.00 28.34      D
ATOM   6528  CD  LYS D 369     110.159 -20.280  26.431  0.00 28.71      D
ATOM   6529  CE  LYS D 369     109.692 -19.395  25.288  0.00 29.07      D
ATOM   6530  NZ  LYS D 369     108.385 -19.851  24.737  0.00 29.21      D
ATOM   6531  C   LYS D 369     113.815 -17.602  27.170  1.00 28.21      D
```

```
ATOM   6532  O   LYS D 369     114.404 -18.432  26.466  1.00 27.80      D
ATOM   6533  N   PHE D 370     114.027 -16.295  27.055  1.00 28.20      D
ATOM   6534  CA  PHE D 370     114.945 -15.779  26.048  1.00 29.53      D
ATOM   6535  CB  PHE D 370     114.804 -14.267  25.930  1.00 30.24      D
ATOM   6536  CG  PHE D 370     115.741 -13.647  24.926  1.00 31.46      D
ATOM   6537  CD1 PHE D 370     117.107 -13.497  25.208  1.00 32.17      D
ATOM   6538  CD2 PHE D 370     115.253 -13.184  23.711  1.00 31.98      D
ATOM   6539  CE1 PHE D 370     117.970 -12.894  24.301  1.00 30.34      D
ATOM   6540  CE2 PHE D 370     116.105 -12.580  22.795  1.00 32.40      D
ATOM   6541  CZ  PHE D 370     117.473 -12.434  23.098  1.00 31.69      D
ATOM   6542  C   PHE D 370     116.418 -16.125  26.250  1.00 29.47      D
ATOM   6543  O   PHE D 370     116.990 -15.909  27.323  1.00 30.76      D
ATOM   6544  N   VAL D 371     117.038 -16.623  25.186  1.00 28.02      D
ATOM   6545  CA  VAL D 371     118.441 -16.986  25.252  1.00 27.30      D
ATOM   6546  CB  VAL D 371     118.648 -18.446  24.756  1.00 26.04      D
ATOM   6547  CG1 VAL D 371     120.104 -18.829  24.825  1.00 22.81      D
ATOM   6548  CG2 VAL D 371     117.827 -19.396  25.624  1.00 22.71      D
ATOM   6549  C   VAL D 371     119.309 -15.995  24.469  1.00 28.27      D
ATOM   6550  O   VAL D 371     119.221 -15.880  23.248  1.00 27.93      D
ATOM   6551  N   PRO D 372     120.161 -15.251  25.188  1.00 29.70      D
ATOM   6552  CD  PRO D 372     120.326 -15.276  26.648  1.00 29.18      D
ATOM   6553  CA  PRO D 372     121.057 -14.258  24.597  1.00 31.17      D
ATOM   6554  CB  PRO D 372     121.744 -13.642  25.816  1.00 29.97      D
ATOM   6555  CG  PRO D 372     120.796 -13.886  26.914  1.00 30.31      D
ATOM   6556  C   PRO D 372     122.071 -14.884  23.659  1.00 32.23      D
ATOM   6557  O   PRO D 372     122.136 -16.104  23.515  1.00 33.92      D
ATOM   6558  N   GLN D 373     122.860 -14.033  23.019  1.00 32.64      D
ATOM   6559  CA  GLN D 373     123.907 -14.511  22.144  1.00 31.91      D
ATOM   6560  CB  GLN D 373     123.945 -13.701  20.865  1.00 31.03      D
ATOM   6561  CG  GLN D 373     124.881 -14.279  19.845  1.00 31.69      D
ATOM   6562  CD  GLN D 373     125.575 -13.202  19.069  1.00 32.49      D
ATOM   6563  OE1 GLN D 373     124.937 -12.328  18.502  1.00 33.06      D
ATOM   6564  NE2 GLN D 373     126.892 -13.251  19.045  1.00 34.46      D
ATOM   6565  C   GLN D 373     125.203 -14.315  22.925  1.00 31.35      D
ATOM   6566  O   GLN D 373     125.612 -13.192  23.224  1.00 31.52      D
ATOM   6567  N   ARG D 374     125.842 -15.418  23.264  1.00 29.71      D
ATOM   6568  CA  ARG D 374     127.059 -15.342  24.024  1.00 29.87      D
ATOM   6569  CB  ARG D 374     127.054 -16.417  25.102  1.00 30.39      D
ATOM   6570  CG  ARG D 374     128.347 -16.511  25.854  1.00 31.03      D
ATOM   6571  CD  ARG D 374     128.261 -17.597  26.873  1.00 31.27      D
ATOM   6572  NE  ARG D 374     129.475 -17.599  27.658  1.00 32.88      D
ATOM   6573  CZ  ARG D 374     129.738 -18.450  28.637  1.00 33.11      D
ATOM   6574  NH1 ARG D 374     128.856 -19.390  28.956  1.00 31.68      D
ATOM   6575  NH2 ARG D 374     130.889 -18.343  29.301  1.00 33.83      D
ATOM   6576  C   ARG D 374     128.306 -15.477  23.161  1.00 30.20      D
ATOM   6577  O   ARG D 374     128.383 -16.319  22.268  1.00 30.52      D
ATOM   6578  N   THR D 375     129.298 -14.654  23.463  1.00 30.06      D
ATOM   6579  CA  THR D 375     130.543 -14.641  22.724  1.00 29.07      D
ATOM   6580  CB  THR D 375     130.574 -13.423  21.801  1.00 29.18      D
ATOM   6581  OG1 THR D 375     129.254 -13.177  21.294  1.00 30.22      D
ATOM   6582  CG2 THR D 375     131.520 -13.650  20.650  1.00 27.55      D
ATOM   6583  C   THR D 375     131.666 -14.506  23.749  1.00 29.99      D
ATOM   6584  O   THR D 375     131.743 -13.505  24.473  1.00 30.81      D
ATOM   6585  N   THR D 376     132.537 -15.504  23.824  1.00 29.02      D
```

```
ATOM   6586  CA  THR D 376     133.631 -15.459  24.789  1.00 28.35      D
ATOM   6587  CB  THR D 376     133.775 -16.810  25.551  1.00 26.89      D
ATOM   6588  OG1 THR D 376     132.516 -17.174  26.129  1.00 24.67      D
ATOM   6589  CG2 THR D 376     134.822 -16.700  26.648  1.00 25.06      D
ATOM   6590  C   THR D 376     134.959 -15.155  24.120  1.00 29.32      D
ATOM   6591  O   THR D 376     135.386 -15.886  23.234  1.00 28.86      D
ATOM   6592  N   LEU D 377     135.616 -14.081  24.555  1.00 31.19      D
ATOM   6593  CA  LEU D 377     136.916 -13.701  24.001  1.00 33.04      D
ATOM   6594  CB  LEU D 377     136.888 -12.242  23.558  1.00 31.62      D
ATOM   6595  CG  LEU D 377     135.621 -11.843  22.793  1.00 32.74      D
ATOM   6596  CD1 LEU D 377     135.718 -10.396  22.376  1.00 32.01      D
ATOM   6597  CD2 LEU D 377     135.430 -12.735  21.590  1.00 32.02      D
ATOM   6598  C   LEU D 377     138.006 -13.907  25.044  1.00 35.05      D
ATOM   6599  O   LEU D 377     137.733 -13.877  26.241  1.00 36.55      D
ATOM   6600  N   ARG D 378     139.238 -14.122  24.590  1.00 37.30      D
ATOM   6601  CA  ARG D 378     140.381 -14.341  25.487  1.00 38.75      D
ATOM   6602  CB  ARG D 378     141.620 -14.732  24.661  1.00 41.44      D
ATOM   6603  CG  ARG D 378     142.735 -15.467  25.412  1.00 45.29      D
ATOM   6604  CD  ARG D 378     143.962 -15.705  24.499  1.00 49.27      D
ATOM   6605  NE  ARG D 378     144.615 -14.445  24.116  1.00 53.86      D
ATOM   6606  CZ  ARG D 378     145.636 -14.322  23.260  1.00 55.92      D
ATOM   6607  NH1 ARG D 378     146.147 -15.400  22.666  1.00 55.78      D
ATOM   6608  NH2 ARG D 378     146.152 -13.109  23.009  1.00 55.08      D
ATOM   6609  C   ARG D 378     140.663 -13.056  26.259  1.00 38.43      D
ATOM   6610  O   ARG D 378     140.498 -11.956  25.723  1.00 37.88      D
ATOM   6611  N   GLY D 379     141.098 -13.206  27.510  1.00 38.54      D
ATOM   6612  CA  GLY D 379     141.408 -12.058  28.349  1.00 38.37      D
ATOM   6613  C   GLY D 379     142.901 -11.817  28.563  1.00 38.46      D
ATOM   6614  O   GLY D 379     143.704 -12.014  27.646  1.00 39.93      D
ATOM   6615  N   HIS D 380     143.270 -11.390  29.771  1.00 36.54      D
ATOM   6616  CA  HIS D 380     144.663 -11.116  30.118  1.00 35.40      D
ATOM   6617  CB  HIS D 380     144.735 -10.098  31.259  1.00 32.54      D
ATOM   6618  CG  HIS D 380     144.169  -8.762  30.910  1.00 29.64      D
ATOM   6619  CD2 HIS D 380     144.748  -7.541  30.837  1.00 29.11      D
ATOM   6620  ND1 HIS D 380     142.845  -8.580  30.581  1.00 28.66      D
ATOM   6621  CE1 HIS D 380     142.630  -7.302  30.323  1.00 26.84      D
ATOM   6622  NE2 HIS D 380     143.768  -6.650  30.470  1.00 28.50      D
ATOM   6623  C   HIS D 380     145.400 -12.389  30.524  1.00 35.86      D
ATOM   6624  O   HIS D 380     144.796 -13.450  30.606  1.00 35.08      D
ATOM   6625  N   MSE D 381     146.699 -12.287  30.790  1.00 37.57      D
ATOM   6626  CA  MSE D 381     147.467 -13.465  31.172  1.00 40.68      D
ATOM   6627  CB  MSE D 381     148.937 -13.253  30.850  1.00 42.82      D
ATOM   6628  CG  MSE D 381     149.177 -13.111  29.372  1.00 45.44      D
ATOM   6629  SE  MSE D 381     150.909 -12.445  28.929  1.00 55.08      D
ATOM   6630  CE  MSE D 381     150.582 -10.533  29.001  1.00 48.67      D
ATOM   6631  C   MSE D 381     147.306 -13.812  32.645  1.00 41.59      D
ATOM   6632  O   MSE D 381     147.979 -14.701  33.169  1.00 40.94      D
ATOM   6633  N   THR D 382     146.392 -13.103  33.296  1.00 42.55      D
ATOM   6634  CA  THR D 382     146.091 -13.286  34.704  1.00 42.91      D
ATOM   6635  CB  THR D 382     146.571 -12.035  35.487  1.00 42.87      D
ATOM   6636  OG1 THR D 382     146.096 -12.083  36.838  1.00 47.41      D
ATOM   6637  CG2 THR D 382     146.091 -10.770  34.806  1.00 42.47      D
ATOM   6638  C   THR D 382     144.566 -13.490  34.809  1.00 42.80      D
ATOM   6639  O   THR D 382     143.799 -12.695  34.280  1.00 45.02      D
```

```
ATOM   6640  N   SER D 383     144.129 -14.559  35.466  1.00 41.05      D
ATOM   6641  CA  SER D 383     142.708 -14.855  35.590  1.00 40.03      D
ATOM   6642  CB  SER D 383     142.527 -16.201  36.285  1.00 41.63      D
ATOM   6643  OG  SER D 383     143.273 -16.252  37.491  1.00 42.67      D
ATOM   6644  C   SER D 383     141.888 -13.806  36.323  1.00 38.85      D
ATOM   6645  O   SER D 383     140.701 -14.007  36.569  1.00 39.35      D
ATOM   6646  N   VAL D 384     142.514 -12.689  36.665  1.00 37.95      D
ATOM   6647  CA  VAL D 384     141.829 -11.620  37.382  1.00 37.40      D
ATOM   6648  CB  VAL D 384     142.471 -11.414  38.777  1.00 39.34      D
ATOM   6649  CG1 VAL D 384     141.606 -10.515  39.638  1.00 39.21      D
ATOM   6650  CG2 VAL D 384     142.672 -12.756  39.451  1.00 41.87      D
ATOM   6651  C   VAL D 384     141.899 -10.302  36.615  1.00 35.77      D
ATOM   6652  O   VAL D 384     142.987  -9.824  36.282  1.00 35.80      D
ATOM   6653  N   ILE D 385     140.741  -9.719  36.330  1.00 33.56      D
ATOM   6654  CA  ILE D 385     140.697  -8.445  35.627  1.00 31.75      D
ATOM   6655  CB  ILE D 385     139.503  -8.347  34.670  1.00 32.21      D
ATOM   6656  CG2 ILE D 385     139.566  -7.028  33.924  1.00 31.42      D
ATOM   6657  CG1 ILE D 385     139.528  -9.506  33.673  1.00 34.12      D
ATOM   6658  CD1 ILE D 385     140.728  -9.519  32.787  1.00 31.79      D
ATOM   6659  C   ILE D 385     140.524  -7.369  36.681  1.00 29.87      D
ATOM   6660  O   ILE D 385     139.636  -7.468  37.523  1.00 29.33      D
ATOM   6661  N   THR D 386     141.364  -6.341  36.631  1.00 28.00      D
ATOM   6662  CA  THR D 386     141.284  -5.262  37.603  1.00 26.59      D
ATOM   6663  CB  THR D 386     142.665  -4.709  37.933  1.00 28.33      D
ATOM   6664  OG1 THR D 386     143.147  -3.965  36.810  1.00 33.14      D
ATOM   6665  CG2 THR D 386     143.629  -5.847  38.258  1.00 27.95      D
ATOM   6666  C   THR D 386     140.370  -4.095  37.219  1.00 23.96      D
ATOM   6667  O   THR D 386     140.049  -3.258  38.057  1.00 23.82      D
ATOM   6668  N   CYS D 387     139.969  -4.000  35.959  1.00 21.99      D
ATOM   6669  CA  CYS D 387     139.032  -2.946  35.583  1.00 21.32      D
ATOM   6670  CB  CYS D 387     139.593  -1.554  35.810  1.00 21.52      D
ATOM   6671  SG  CYS D 387     141.286  -1.370  35.494  1.00 24.48      D
ATOM   6672  C   CYS D 387     138.522  -3.058  34.185  1.00 20.32      D
ATOM   6673  O   CYS D 387     139.180  -3.609  33.309  1.00 20.62      D
ATOM   6674  N   LEU D 388     137.313  -2.554  33.993  1.00 21.13      D
ATOM   6675  CA  LEU D 388     136.666  -2.620  32.699  1.00 21.99      D
ATOM   6676  CB  LEU D 388     135.720  -3.811  32.699  1.00 19.44      D
ATOM   6677  CG  LEU D 388     134.666  -3.896  31.603  1.00 17.83      D
ATOM   6678  CD1 LEU D 388     134.369  -5.364  31.382  1.00 19.58      D
ATOM   6679  CD2 LEU D 388     133.406  -3.172  32.009  1.00 17.27      D
ATOM   6680  C   LEU D 388     135.910  -1.349  32.307  1.00 23.54      D
ATOM   6681  O   LEU D 388     135.262  -0.724  33.136  1.00 24.86      D
ATOM   6682  N   GLN D 389     136.011  -0.965  31.038  1.00 25.33      D
ATOM   6683  CA  GLN D 389     135.302   0.203  30.521  1.00 25.28      D
ATOM   6684  CB  GLN D 389     136.275   1.296  30.073  1.00 25.97      D
ATOM   6685  CG  GLN D 389     137.029   2.071  31.150  1.00 25.10      D
ATOM   6686  CD  GLN D 389     136.179   3.114  31.877  1.00 26.41      D
ATOM   6687  OE1 GLN D 389     135.673   2.850  32.949  1.00 26.25      D
ATOM   6688  NE2 GLN D 389     136.031   4.304  31.293  1.00 27.94      D
ATOM   6689  C   GLN D 389     134.477  -0.233  29.303  1.00 26.25      D
ATOM   6690  O   GLN D 389     134.917  -1.076  28.515  1.00 26.39      D
ATOM   6691  N   PHE D 390     133.284   0.340  29.153  1.00 27.94      D
ATOM   6692  CA  PHE D 390     132.415   0.045  28.015  1.00 28.91      D
ATOM   6693  CB  PHE D 390     131.364  -0.995  28.424  1.00 26.05      D
```

```
ATOM   6694  CG  PHE D 390     130.416  -1.381  27.322  1.00 26.58      D
ATOM   6695  CD1 PHE D 390     130.826  -1.411  25.998  1.00 27.31      D
ATOM   6696  CD2 PHE D 390     129.087  -1.675  27.609  1.00 27.25      D
ATOM   6697  CE1 PHE D 390     129.921  -1.716  24.978  1.00 26.45      D
ATOM   6698  CE2 PHE D 390     128.179  -1.982  26.595  1.00 26.66      D
ATOM   6699  CZ  PHE D 390     128.597  -1.999  25.284  1.00 25.88      D
ATOM   6700  C   PHE D 390     131.800   1.375  27.521  1.00 31.17      D
ATOM   6701  O   PHE D 390     130.844   1.911  28.095  1.00 31.73      D
ATOM   6702  N   GLU D 391     132.404   1.908  26.460  1.00 33.23      D
ATOM   6703  CA  GLU D 391     132.004   3.172  25.842  1.00 36.52      D
ATOM   6704  CB  GLU D 391     132.752   4.335  26.494  1.00 37.25      D
ATOM   6705  CG  GLU D 391     131.870   5.425  27.041  1.00 38.77      D
ATOM   6706  CD  GLU D 391     131.258   5.032  28.354  1.00 39.09      D
ATOM   6707  OE1 GLU D 391     132.023   4.888  29.322  1.00 40.49      D
ATOM   6708  OE2 GLU D 391     130.024   4.859  28.417  1.00 39.48      D
ATOM   6709  C   GLU D 391     132.377   3.150  24.360  1.00 37.92      D
ATOM   6710  O   GLU D 391     133.293   2.426  23.956  1.00 39.21      D
ATOM   6711  N   ASP D 392     131.704   3.971  23.557  1.00 38.58      D
ATOM   6712  CA  ASP D 392     131.986   4.053  22.112  1.00 38.07      D
ATOM   6713  CB  ASP D 392     133.157   5.009  21.858  1.00 37.43      D
ATOM   6714  CG  ASP D 392     132.716   6.428  21.778  1.00 39.32      D
ATOM   6715  OD1 ASP D 392     131.501   6.650  21.954  1.00 40.76      D
ATOM   6716  OD2 ASP D 392     133.557   7.317  21.530  1.00 40.53      D
ATOM   6717  C   ASP D 392     132.253   2.725  21.400  1.00 36.82      D
ATOM   6718  O   ASP D 392     133.221   2.589  20.647  1.00 36.96      D
ATOM   6719  N   ASN D 393     131.381   1.753  21.631  1.00 35.81      D
ATOM   6720  CA  ASN D 393     131.513   0.448  21.000  1.00 36.51      D
ATOM   6721  CB  ASN D 393     131.410   0.572  19.471  1.00 37.62      D
ATOM   6722  CG  ASN D 393     130.111   1.264  19.001  1.00 39.78      D
ATOM   6723  OD1 ASN D 393     130.023   1.696  17.846  1.00 41.53      D
ATOM   6724  ND2 ASN D 393     129.111   1.362  19.881  1.00 38.28      D
ATOM   6725  C   ASN D 393     132.829  -0.215  21.366  1.00 34.65      D
ATOM   6726  O   ASN D 393     133.249  -1.163  20.710  1.00 34.87      D
ATOM   6727  N   TYR D 394     133.477   0.292  22.409  1.00 33.42      D
ATOM   6728  CA  TYR D 394     134.742  -0.264  22.884  1.00 32.37      D
ATOM   6729  CB  TYR D 394     135.783   0.838  23.102  1.00 32.07      D
ATOM   6730  CG  TYR D 394     136.458   1.349  21.860  1.00 32.95      D
ATOM   6731  CD1 TYR D 394     137.124   0.479  20.992  1.00 32.58      D
ATOM   6732  CE1 TYR D 394     137.777   0.953  19.858  1.00 31.50      D
ATOM   6733  CD2 TYR D 394     136.459   2.704  21.565  1.00 31.89      D
ATOM   6734  CE2 TYR D 394     137.104   3.189  20.445  1.00 33.06      D
ATOM   6735  CZ  TYR D 394     137.762   2.316  19.594  1.00 33.32      D
ATOM   6736  OH  TYR D 394     138.406   2.827  18.492  1.00 33.69      D
ATOM   6737  C   TYR D 394     134.554  -0.956  24.224  1.00 32.16      D
ATOM   6738  O   TYR D 394     133.692  -0.582  25.016  1.00 33.01      D
ATOM   6739  N   VAL D 395     135.359  -1.970  24.481  1.00 31.18      D
ATOM   6740  CA  VAL D 395     135.307  -2.636  25.767  1.00 30.34      D
ATOM   6741  CB  VAL D 395     134.724  -4.036  25.689  1.00 32.30      D
ATOM   6742  CG1 VAL D 395     134.537  -4.571  27.092  1.00 30.09      D
ATOM   6743  CG2 VAL D 395     133.388  -4.017  24.945  1.00 32.97      D
ATOM   6744  C   VAL D 395     136.751  -2.752  26.150  1.00 29.50      D
ATOM   6745  O   VAL D 395     137.469  -3.592  25.608  1.00 30.47      D
ATOM   6746  N   ILE D 396     137.190  -1.895  27.061  1.00 27.33      D
ATOM   6747  CA  ILE D 396     138.579  -1.929  27.471  1.00 24.79      D
```

```
ATOM   6748  CB  ILE D 396     139.202  -0.529  27.477  1.00 20.54      D
ATOM   6749  CG2 ILE D 396     140.724  -0.654  27.607  1.00 18.18      D
ATOM   6750  CG1 ILE D 396     138.779   0.231  26.222  1.00 19.10      D
ATOM   6751  CD1 ILE D 396     137.698   1.261  26.480  1.00 15.50      D
ATOM   6752  C   ILE D 396     138.721  -2.532  28.860  1.00 25.91      D
ATOM   6753  O   ILE D 396     137.839  -2.371  29.709  1.00 25.28      D
ATOM   6754  N   THR D 397     139.839  -3.228  29.075  1.00 25.38      D
ATOM   6755  CA  THR D 397     140.133  -3.867  30.352  1.00 24.35      D
ATOM   6756  CB  THR D 397     139.734  -5.353  30.367  1.00 23.41      D
ATOM   6757  OG1 THR D 397     140.542  -6.067  29.425  1.00 22.79      D
ATOM   6758  CG2 THR D 397     138.280  -5.530  30.010  1.00 22.25      D
ATOM   6759  C   THR D 397     141.610  -3.834  30.732  1.00 25.66      D
ATOM   6760  O   THR D 397     142.492  -3.945  29.876  1.00 25.23      D
ATOM   6761  N   GLY D 398     141.871  -3.715  32.032  1.00 26.89      D
ATOM   6762  CA  GLY D 398     143.239  -3.717  32.535  1.00 27.00      D
ATOM   6763  C   GLY D 398     143.440  -4.892  33.487  1.00 26.90      D
ATOM   6764  O   GLY D 398     142.464  -5.481  33.951  1.00 26.42      D
ATOM   6765  N   ALA D 399     144.692  -5.250  33.776  1.00 28.42      D
ATOM   6766  CA  ALA D 399     144.977  -6.367  34.694  1.00 29.91      D
ATOM   6767  CB  ALA D 399     144.889  -7.701  33.945  1.00 28.40      D
ATOM   6768  C   ALA D 399     146.335  -6.265  35.410  1.00 31.06      D
ATOM   6769  O   ALA D 399     147.208  -5.469  35.041  1.00 29.92      D
ATOM   6770  N   ASP D 400     146.511  -7.083  36.444  1.00 33.65      D
ATOM   6771  CA  ASP D 400     147.767  -7.066  37.178  1.00 35.36      D
ATOM   6772  CB  ASP D 400     147.670  -7.891  38.473  1.00 37.51      D
ATOM   6773  CG  ASP D 400     148.845  -7.626  39.429  1.00 42.78      D
ATOM   6774  OD1 ASP D 400     149.073  -6.446  39.813  1.00 42.00      D
ATOM   6775  OD2 ASP D 400     149.544  -8.603  39.802  1.00 45.77      D
ATOM   6776  C   ASP D 400     148.818  -7.639  36.237  1.00 34.42      D
ATOM   6777  O   ASP D 400     149.996  -7.735  36.579  1.00 34.18      D
ATOM   6778  N   ASP D 401     148.379  -8.014  35.037  1.00 33.68      D
ATOM   6779  CA  ASP D 401     149.293  -8.550  34.047  1.00 32.54      D
ATOM   6780  CB  ASP D 401     148.571  -9.554  33.118  1.00 31.92      D
ATOM   6781  CG  ASP D 401     147.897  -8.910  31.909  1.00 31.59      D
ATOM   6782  OD1 ASP D 401     147.579  -7.704  31.945  1.00 30.42      D
ATOM   6783  OD2 ASP D 401     147.671  -9.645  30.916  1.00 31.10      D
ATOM   6784  C   ASP D 401     149.901  -7.372  33.293  1.00 32.98      D
ATOM   6785  O   ASP D 401     150.551  -7.539  32.266  1.00 33.47      D
ATOM   6786  N   LYS D 402     149.699  -6.180  33.854  1.00 33.97      D
ATOM   6787  CA  LYS D 402     150.215  -4.921  33.319  1.00 34.64      D
ATOM   6788  CB  LYS D 402     151.735  -4.825  33.568  1.00 33.75      D
ATOM   6789  CG  LYS D 402     152.545  -5.988  33.073  1.00 33.34      D
ATOM   6790  CD  LYS D 402     153.625  -6.377  34.058  1.00 34.65      D
ATOM   6791  CE  LYS D 402     154.661  -5.300  34.221  1.00 35.08      D
ATOM   6792  NZ  LYS D 402     155.714  -5.811  35.142  1.00 34.72      D
ATOM   6793  C   LYS D 402     149.895  -4.650  31.846  1.00 35.07      D
ATOM   6794  O   LYS D 402     150.606  -3.907  31.167  1.00 35.57      D
ATOM   6795  N   MSE D 403     148.809  -5.238  31.360  1.00 37.46      D
ATOM   6796  CA  MSE D 403     148.389  -5.066  29.966  1.00 39.42      D
ATOM   6797  CB  MSE D 403     148.429  -6.405  29.210  1.00 40.61      D
ATOM   6798  CG  MSE D 403     149.792  -7.054  29.119  1.00 42.82      D
ATOM   6799  SE  MSE D 403     150.956  -5.997  28.018  1.00 47.96      D
ATOM   6800  CE  MSE D 403     152.415  -5.649  29.261  1.00 46.83      D
ATOM   6801  C   MSE D 403     146.970  -4.518  29.882  1.00 39.22      D
```

```
ATOM   6802  O   MSE D 403     146.140  -4.767  30.761  1.00 41.64      D
ATOM   6803  N   ILE D 404     146.691  -3.797  28.802  1.00 37.92      D
ATOM   6804  CA  ILE D 404     145.372  -3.216  28.582  1.00 35.96      D
ATOM   6805  CB  ILE D 404     145.455  -1.675  28.574  1.00 34.69      D
ATOM   6806  CG2 ILE D 404     144.114  -1.082  28.156  1.00 33.19      D
ATOM   6807  CG1 ILE D 404     145.880  -1.186  29.962  1.00 33.10      D
ATOM   6808  CD1 ILE D 404     146.272   0.266  29.999  1.00 31.33      D
ATOM   6809  C   ILE D 404     144.788  -3.709  27.251  1.00 35.14      D
ATOM   6810  O   ILE D 404     145.304  -3.392  26.193  1.00 34.48      D
ATOM   6811  N   ARG D 405     143.709  -4.482  27.325  1.00 34.81      D
ATOM   6812  CA  ARG D 405     143.046  -5.027  26.151  1.00 34.51      D
ATOM   6813  CB  ARG D 405     142.428  -6.373  26.494  1.00 34.25      D
ATOM   6814  CG  ARG D 405     143.353  -7.285  27.227  1.00 34.29      D
ATOM   6815  CD  ARG D 405     144.147  -8.101  26.302  1.00 33.92      D
ATOM   6816  NE  ARG D 405     143.362  -9.187  25.745  1.00 34.85      D
ATOM   6817  CZ  ARG D 405     143.844 -10.076  24.882  1.00 37.01      D
ATOM   6818  NH1 ARG D 405     145.110  -9.992  24.481  1.00 32.55      D
ATOM   6819  NH2 ARG D 405     143.069 -11.063  24.436  1.00 38.58      D
ATOM   6820  C   ARG D 405     141.931  -4.099  25.668  1.00 35.40      D
ATOM   6821  O   ARG D 405     141.238  -3.474  26.479  1.00 36.54      D
ATOM   6822  N   VAL D 406     141.749  -4.041  24.349  1.00 35.29      D
ATOM   6823  CA  VAL D 406     140.719  -3.214  23.719  1.00 34.73      D
ATOM   6824  CB  VAL D 406     141.332  -2.093  22.879  1.00 35.48      D
ATOM   6825  CG1 VAL D 406     140.229  -1.244  22.275  1.00 35.19      D
ATOM   6826  CG2 VAL D 406     142.275  -1.253  23.737  1.00 35.51      D
ATOM   6827  C   VAL D 406     139.921  -4.085  22.780  1.00 34.43      D
ATOM   6828  O   VAL D 406     140.500  -4.664  21.874  1.00 34.33      D
ATOM   6829  N   TYR D 407     138.603  -4.160  22.977  1.00 34.53      D
ATOM   6830  CA  TYR D 407     137.739  -4.985  22.124  1.00 34.18      D
ATOM   6831  CB  TYR D 407     137.059  -6.091  22.937  1.00 33.29      D
ATOM   6832  CG  TYR D 407     137.966  -6.948  23.781  1.00 33.16      D
ATOM   6833  CD1 TYR D 407     138.423  -6.509  25.026  1.00 32.93      D
ATOM   6834  CE1 TYR D 407     139.255  -7.313  25.802  1.00 33.43      D
ATOM   6835  CD2 TYR D 407     138.362  -8.206  23.335  1.00 31.85      D
ATOM   6836  CE2 TYR D 407     139.189  -9.013  24.091  1.00 31.74      D
ATOM   6837  CZ  TYR D 407     139.637  -8.572  25.320  1.00 33.54      D
ATOM   6838  OH  TYR D 407     140.485  -9.378  26.052  1.00 34.77      D
ATOM   6839  C   TYR D 407     136.635  -4.194  21.417  1.00 34.58      D
ATOM   6840  O   TYR D 407     136.246  -3.117  21.864  1.00 35.32      D
ATOM   6841  N   ASP D 408     136.122  -4.775  20.332  1.00 35.38      D
ATOM   6842  CA  ASP D 408     135.043  -4.221  19.501  1.00 35.74      D
ATOM   6843  CB  ASP D 408     135.302  -4.625  18.038  1.00 38.38      D
ATOM   6844  CG  ASP D 408     134.214  -4.143  17.066  1.00 40.45      D
ATOM   6845  OD1 ASP D 408     133.015  -4.143  17.433  1.00 41.61      D
ATOM   6846  OD2 ASP D 408     134.563  -3.781  15.917  1.00 39.05      D
ATOM   6847  C   ASP D 408     133.685  -4.788  19.965  1.00 35.67      D
ATOM   6848  O   ASP D 408     133.413  -5.980  19.799  1.00 35.45      D
ATOM   6849  N   SER D 409     132.829  -3.934  20.519  1.00 36.24      D
ATOM   6850  CA  SER D 409     131.510  -4.351  21.021  1.00 37.97      D
ATOM   6851  CB  SER D 409     130.779  -3.160  21.623  1.00 39.00      D
ATOM   6852  OG  SER D 409     131.590  -2.452  22.533  1.00 42.40      D
ATOM   6853  C   SER D 409     130.594  -4.953  19.968  1.00 39.04      D
ATOM   6854  O   SER D 409     129.915  -5.958  20.216  1.00 38.64      D
ATOM   6855  N   ILE D 410     130.565  -4.295  18.807  1.00 40.27      D
```

```
ATOM   6856  CA  ILE D 410     129.740  -4.695  17.658  1.00 41.19      D
ATOM   6857  CB  ILE D 410     129.743  -3.613  16.553  1.00 42.29      D
ATOM   6858  CG2 ILE D 410     128.654  -3.904  15.539  1.00 41.48      D
ATOM   6859  CG1 ILE D 410     129.507  -2.227  17.162  1.00 43.94      D
ATOM   6860  CD1 ILE D 410     129.838  -1.089  16.202  1.00 43.04      D
ATOM   6861  C   ILE D 410     130.244  -5.996  17.038  1.00 40.21      D
ATOM   6862  O   ILE D 410     129.616  -7.041  17.170  1.00 40.47      D
ATOM   6863  N   ASN D 411     131.385  -5.945  16.370  1.00 38.97      D
ATOM   6864  CA  ASN D 411     131.900  -7.153  15.769  1.00 39.16      D
ATOM   6865  CB  ASN D 411     133.158  -6.848  14.985  1.00 41.69      D
ATOM   6866  CG  ASN D 411     132.943  -5.731  13.995  1.00 43.77      D
ATOM   6867  OD1 ASN D 411     131.889  -5.649  13.355  1.00 43.07      D
ATOM   6868  ND2 ASN D 411     133.938  -4.866  13.855  1.00 45.58      D
ATOM   6869  C   ASN D 411     132.178  -8.213  16.805  1.00 38.20      D
ATOM   6870  O   ASN D 411     132.364  -9.377  16.458  1.00 36.34      D
ATOM   6871  N   LYS D 412     132.197  -7.800  18.074  1.00 37.74      D
ATOM   6872  CA  LYS D 412     132.451  -8.693  19.211  1.00 36.63      D
ATOM   6873  CB  LYS D 412     131.300  -9.690  19.338  1.00 35.83      D
ATOM   6874  CG  LYS D 412     129.936  -9.018  19.314  1.00 35.16      D
ATOM   6875  CD  LYS D 412     128.805 -10.011  19.175  1.00 34.88      D
ATOM   6876  CE  LYS D 412     127.483  -9.278  19.119  1.00 36.26      D
ATOM   6877  NZ  LYS D 412     126.321 -10.211  19.101  1.00 37.05      D
ATOM   6878  C   LYS D 412     133.776  -9.442  19.066  1.00 36.14      D
ATOM   6879  O   LYS D 412     133.828 -10.659  19.227  1.00 35.34      D
ATOM   6880  N   LYS D 413     134.845  -8.707  18.772  1.00 36.48      D
ATOM   6881  CA  LYS D 413     136.161  -9.314  18.597  1.00 38.12      D
ATOM   6882  CB  LYS D 413     136.440  -9.573  17.118  1.00 37.83      D
ATOM   6883  CG  LYS D 413     136.378  -8.322  16.257  1.00 41.43      D
ATOM   6884  CD  LYS D 413     136.964  -8.566  14.853  1.00 44.72      D
ATOM   6885  CE  LYS D 413     136.674  -7.400  13.885  1.00 46.65      D
ATOM   6886  NZ  LYS D 413     137.132  -6.056  14.371  1.00 47.55      D
ATOM   6887  C   LYS D 413     137.303  -8.471  19.159  1.00 38.78      D
ATOM   6888  O   LYS D 413     137.244  -7.242  19.151  1.00 38.60      D
ATOM   6889  N   PHE D 414     138.348  -9.149  19.630  1.00 38.98      D
ATOM   6890  CA  PHE D 414     139.520  -8.489  20.191  1.00 38.98      D
ATOM   6891  CB  PHE D 414     140.513  -9.528  20.715  1.00 39.56      D
ATOM   6892  CG  PHE D 414     141.908  -8.997  20.902  1.00 41.07      D
ATOM   6893  CD1 PHE D 414     142.184  -8.046  21.874  1.00 43.51      D
ATOM   6894  CD2 PHE D 414     142.949  -9.454  20.110  1.00 41.71      D
ATOM   6895  CE1 PHE D 414     143.488  -7.557  22.058  1.00 44.32      D
ATOM   6896  CE2 PHE D 414     144.251  -8.973  20.287  1.00 43.60      D
ATOM   6897  CZ  PHE D 414     144.519  -8.022  21.264  1.00 42.78      D
ATOM   6898  C   PHE D 414     140.208  -7.620  19.157  1.00 39.17      D
ATOM   6899  O   PHE D 414     140.529  -8.083  18.068  1.00 40.84      D
ATOM   6900  N   LEU D 415     140.430  -6.359  19.506  1.00 38.34      D
ATOM   6901  CA  LEU D 415     141.099  -5.434  18.617  1.00 37.48      D
ATOM   6902  CB  LEU D 415     140.555  -4.026  18.815  1.00 37.15      D
ATOM   6903  CG  LEU D 415     139.163  -3.792  18.224  1.00 38.52      D
ATOM   6904  CD1 LEU D 415     138.737  -2.351  18.453  1.00 39.38      D
ATOM   6905  CD2 LEU D 415     139.191  -4.091  16.736  1.00 39.17      D
ATOM   6906  C   LEU D 415     142.611  -5.451  18.832  1.00 37.67      D
ATOM   6907  O   LEU D 415     143.328  -6.171  18.138  1.00 38.98      D
ATOM   6908  N   LEU D 416     143.097  -4.681  19.799  1.00 35.95      D
ATOM   6909  CA  LEU D 416     144.528  -4.611  20.052  1.00 34.61      D
```

```
ATOM   6910  CB  LEU D 416     145.102  -3.394  19.317  1.00 32.51      D
ATOM   6911  CG  LEU D 416     144.656  -2.045  19.880  1.00 30.50      D
ATOM   6912  CD1 LEU D 416     145.700  -1.579  20.853  1.00 31.53      D
ATOM   6913  CD2 LEU D 416     144.470  -1.017  18.789  1.00 30.55      D
ATOM   6914  C   LEU D 416     144.865  -4.519  21.545  1.00 35.53      D
ATOM   6915  O   LEU D 416     144.013  -4.200  22.364  1.00 36.55      D
ATOM   6916  N   GLN D 417     146.116  -4.791  21.891  1.00 35.81      D
ATOM   6917  CA  GLN D 417     146.547  -4.716  23.271  1.00 35.57      D
ATOM   6918  CB  GLN D 417     147.254  -6.007  23.671  1.00 37.43      D
ATOM   6919  CG  GLN D 417     147.625  -6.074  25.145  1.00 39.62      D
ATOM   6920  CD  GLN D 417     148.512  -7.253  25.464  1.00 41.04      D
ATOM   6921  OE1 GLN D 417     149.615  -7.378  24.914  1.00 43.24      D
ATOM   6922  NE2 GLN D 417     148.046  -8.128  26.358  1.00 40.41      D
ATOM   6923  C   GLN D 417     147.506  -3.532  23.450  1.00 35.61      D
ATOM   6924  O   GLN D 417     148.374  -3.297  22.605  1.00 35.43      D
ATOM   6925  N   LEU D 418     147.337  -2.798  24.551  1.00 35.15      D
ATOM   6926  CA  LEU D 418     148.166  -1.644  24.885  1.00 33.41      D
ATOM   6927  CB  LEU D 418     147.315  -0.523  25.429  1.00 31.33      D
ATOM   6928  CG  LEU D 418     146.413   0.034  24.359  1.00 31.84      D
ATOM   6929  CD1 LEU D 418     145.508   1.119  24.943  1.00 33.02      D
ATOM   6930  CD2 LEU D 418     147.293   0.595  23.253  1.00 33.13      D
ATOM   6931  C   LEU D 418     149.180  -2.006  25.939  1.00 33.92      D
ATOM   6932  O   LEU D 418     148.811  -2.281  27.076  1.00 33.63      D
ATOM   6933  N   SER D 419     150.458  -1.991  25.572  1.00 35.50      D
ATOM   6934  CA  SER D 419     151.529  -2.323  26.518  1.00 35.75      D
ATOM   6935  CB  SER D 419     152.504  -3.304  25.889  1.00 36.24      D
ATOM   6936  OG  SER D 419     153.366  -2.611  25.006  1.00 39.10      D
ATOM   6937  C   SER D 419     152.286  -1.060  26.903  1.00 34.65      D
ATOM   6938  O   SER D 419     152.148  -0.036  26.243  1.00 35.71      D
ATOM   6939  N   GLY D 420     153.082  -1.132  27.969  1.00 34.21      D
ATOM   6940  CA  GLY D 420     153.845   0.030  28.407  1.00 32.81      D
ATOM   6941  C   GLY D 420     154.127   0.063  29.904  1.00 32.19      D
ATOM   6942  O   GLY D 420     155.277   0.111  30.334  1.00 32.95      D
ATOM   6943  N   HIS D 421     153.057   0.038  30.690  1.00 32.53      D
ATOM   6944  CA  HIS D 421     153.116   0.056  32.142  1.00 31.89      D
ATOM   6945  CB  HIS D 421     151.744  -0.233  32.728  1.00 28.17      D
ATOM   6946  CG  HIS D 421     150.862   0.972  32.856  1.00 26.59      D
ATOM   6947  CD2 HIS D 421     149.677   1.270  32.274  1.00 23.86      D
ATOM   6948  ND1 HIS D 421     151.123   1.998  33.738  1.00 24.07      D
ATOM   6949  CE1 HIS D 421     150.133   2.872  33.699  1.00 24.39      D
ATOM   6950  NE2 HIS D 421     149.243   2.454  32.818  1.00 22.81      D
ATOM   6951  C   HIS D 421     154.082  -0.966  32.714  1.00 34.84      D
ATOM   6952  O   HIS D 421     154.005  -2.162  32.399  1.00 35.95      D
ATOM   6953  N   ASP D 422     154.973  -0.487  33.580  1.00 37.06      D
ATOM   6954  CA  ASP D 422     155.969  -1.328  34.241  1.00 37.22      D
ATOM   6955  CB  ASP D 422     157.181  -0.481  34.655  1.00 37.19      D
ATOM   6956  CG  ASP D 422     157.811   0.261  33.479  1.00 38.07      D
ATOM   6957  OD1 ASP D 422     158.398  -0.414  32.605  1.00 36.97      D
ATOM   6958  OD2 ASP D 422     157.716   1.519  33.426  1.00 39.00      D
ATOM   6959  C   ASP D 422     155.331  -1.974  35.468  1.00 37.57      D
ATOM   6960  O   ASP D 422     155.947  -2.791  36.155  1.00 38.18      D
ATOM   6961  N   GLY D 423     154.089  -1.584  35.735  1.00 38.03      D
ATOM   6962  CA  GLY D 423     153.357  -2.135  36.862  1.00 37.36      D
ATOM   6963  C   GLY D 423     151.963  -2.599  36.451  1.00 36.40      D
```

```
ATOM   6964  O   GLY D 423     151.496  -2.282  35.358  1.00 37.00      D
ATOM   6965  N   GLY D 424     151.297  -3.361  37.311  1.00 35.05      D
ATOM   6966  CA  GLY D 424     149.965  -3.823  36.984  1.00 33.45      D
ATOM   6967  C   GLY D 424     149.032  -2.637  36.920  1.00 33.03      D
ATOM   6968  O   GLY D 424     149.183  -1.692  37.687  1.00 32.43      D
ATOM   6969  N   VAL D 425     148.074  -2.685  36.004  1.00 33.29      D
ATOM   6970  CA  VAL D 425     147.112  -1.602  35.826  1.00 34.26      D
ATOM   6971  CB  VAL D 425     146.545  -1.623  34.420  1.00 34.93      D
ATOM   6972  CG1 VAL D 425     145.785  -0.328  34.150  1.00 37.13      D
ATOM   6973  CG2 VAL D 425     147.661  -1.843  33.433  1.00 34.83      D
ATOM   6974  C   VAL D 425     145.955  -1.776  36.795  1.00 33.41      D
ATOM   6975  O   VAL D 425     145.473  -2.880  36.975  1.00 33.61      D
ATOM   6976  N   TRP D 426     145.493  -0.700  37.410  1.00 32.49      D
ATOM   6977  CA  TRP D 426     144.395  -0.837  38.343  1.00 32.03      D
ATOM   6978  CB  TRP D 426     144.952  -0.866  39.774  1.00 30.72      D
ATOM   6979  CG  TRP D 426     145.618  -2.192  40.132  1.00 29.46      D
ATOM   6980  CD2 TRP D 426     145.011  -3.288  40.834  1.00 27.59      D
ATOM   6981  CE2 TRP D 426     145.982  -4.311  40.937  1.00 25.67      D
ATOM   6982  CE3 TRP D 426     143.738  -3.502  41.390  1.00 27.62      D
ATOM   6983  CD1 TRP D 426     146.903  -2.592  39.838  1.00 28.36      D
ATOM   6984  NE1 TRP D 426     147.122  -3.863  40.321  1.00 26.42      D
ATOM   6985  CZ2 TRP D 426     145.720  -5.527  41.572  1.00 23.76      D
ATOM   6986  CZ3 TRP D 426     143.477  -4.712  42.021  1.00 25.66      D
ATOM   6987  CH2 TRP D 426     144.467  -5.711  42.108  1.00 24.10      D
ATOM   6988  C   TRP D 426     143.291   0.224  38.190  1.00 32.39      D
ATOM   6989  O   TRP D 426     142.270   0.182  38.876  1.00 32.60      D
ATOM   6990  N   ALA D 427     143.483   1.164  37.275  1.00 31.70      D
ATOM   6991  CA  ALA D 427     142.489   2.201  37.060  1.00 32.14      D
ATOM   6992  CB  ALA D 427     142.699   3.330  38.059  1.00 30.77      D
ATOM   6993  C   ALA D 427     142.544   2.749  35.631  1.00 32.54      D
ATOM   6994  O   ALA D 427     143.610   3.128  35.148  1.00 33.11      D
ATOM   6995  N   LEU D 428     141.403   2.763  34.949  1.00 31.96      D
ATOM   6996  CA  LEU D 428     141.362   3.298  33.605  1.00 31.52      D
ATOM   6997  CB  LEU D 428     141.879   2.273  32.591  1.00 30.47      D
ATOM   6998  CG  LEU D 428     141.523   0.793  32.619  1.00 25.70      D
ATOM   6999  CD1 LEU D 428     140.061   0.566  32.426  1.00 26.95      D
ATOM   7000  CD2 LEU D 428     142.302   0.127  31.520  1.00 26.15      D
ATOM   7001  C   LEU D 428     139.998   3.823  33.185  1.00 32.41      D
ATOM   7002  O   LEU D 428     139.015   3.092  33.159  1.00 31.99      D
ATOM   7003  N   LYS D 429     139.970   5.117  32.874  1.00 34.44      D
ATOM   7004  CA  LYS D 429     138.779   5.846  32.441  1.00 36.04      D
ATOM   7005  CB  LYS D 429     138.655   7.149  33.247  1.00 36.79      D
ATOM   7006  CG  LYS D 429     137.379   7.954  33.000  1.00 41.16      D
ATOM   7007  CD  LYS D 429     136.228   7.499  33.914  1.00 44.67      D
ATOM   7008  CE  LYS D 429     134.828   7.936  33.399  1.00 47.43      D
ATOM   7009  NZ  LYS D 429     134.385   7.223  32.133  1.00 49.62      D
ATOM   7010  C   LYS D 429     138.944   6.184  30.951  1.00 35.80      D
ATOM   7011  O   LYS D 429     139.982   6.698  30.531  1.00 35.22      D
ATOM   7012  N   TYR D 430     137.926   5.888  30.152  1.00 36.71      D
ATOM   7013  CA  TYR D 430     137.962   6.183  28.719  1.00 38.50      D
ATOM   7014  CB  TYR D 430     137.142   5.152  27.936  1.00 38.31      D
ATOM   7015  CG  TYR D 430     136.840   5.560  26.501  1.00 38.68      D
ATOM   7016  CD1 TYR D 430     135.713   6.331  26.192  1.00 38.18      D
ATOM   7017  CE1 TYR D 430     135.427   6.702  24.875  1.00 37.22      D
```

```
ATOM   7018  CD2 TYR D 430     137.680   5.173  25.449  1.00 39.59      D
ATOM   7019  CE2 TYR D 430     137.403   5.542  24.126  1.00 38.38      D
ATOM   7020  CZ  TYR D 430     136.275   6.303  23.853  1.00 38.21      D
ATOM   7021  OH  TYR D 430     135.983   6.646  22.557  1.00 37.82      D
ATOM   7022  C   TYR D 430     137.401   7.574  28.427  1.00 39.86      D
ATOM   7023  O   TYR D 430     136.344   7.931  28.934  1.00 39.99      D
ATOM   7024  N   ALA D 431     138.109   8.349  27.607  1.00 40.69      D
ATOM   7025  CA  ALA D 431     137.660   9.688  27.227  1.00 41.42      D
ATOM   7026  CB  ALA D 431     138.790  10.695  27.407  1.00 40.10      D
ATOM   7027  C   ALA D 431     137.208   9.641  25.763  1.00 43.09      D
ATOM   7028  O   ALA D 431     137.842   8.998  24.916  1.00 43.69      D
ATOM   7029  N   HIS D 432     136.108  10.321  25.465  1.00 42.71      D
ATOM   7030  CA  HIS D 432     135.584  10.340  24.102  1.00 43.16      D
ATOM   7031  CB  HIS D 432     134.468  11.383  23.966  1.00 47.95      D
ATOM   7032  CG  HIS D 432     133.942  11.523  22.566  1.00 53.08      D
ATOM   7033  CD2 HIS D 432     133.728  12.622  21.801  1.00 53.58      D
ATOM   7034  ND1 HIS D 432     133.594  10.439  21.787  1.00 53.70      D
ATOM   7035  CE1 HIS D 432     133.192  10.865  20.601  1.00 54.74      D
ATOM   7036  NE2 HIS D 432     133.265  12.184  20.584  1.00 54.71      D
ATOM   7037  C   HIS D 432     136.646  10.636  23.052  1.00 40.32      D
ATOM   7038  O   HIS D 432     137.420  11.573  23.201  1.00 40.89      D
ATOM   7039  N   GLY D 433     136.669   9.852  21.980  1.00 37.59      D
ATOM   7040  CA  GLY D 433     137.640  10.095  20.926  1.00 36.16      D
ATOM   7041  C   GLY D 433     138.701   9.029  20.850  1.00 34.81      D
ATOM   7042  O   GLY D 433     139.697   9.177  20.143  1.00 32.92      D
ATOM   7043  N   GLY D 434     138.474   7.948  21.588  1.00 36.25      D
ATOM   7044  CA  GLY D 434     139.412   6.841  21.617  1.00 36.22      D
ATOM   7045  C   GLY D 434     140.580   7.079  22.557  1.00 36.76      D
ATOM   7046  O   GLY D 434     141.559   6.338  22.493  1.00 37.12      D
ATOM   7047  N   ILE D 435     140.469   8.106  23.411  1.00 37.42      D
ATOM   7048  CA  ILE D 435     141.501   8.478  24.397  1.00 37.95      D
ATOM   7049  CB  ILE D 435     141.424   9.992  24.784  1.00 39.16      D
ATOM   7050  CG2 ILE D 435     142.684  10.430  25.539  1.00 37.49      D
ATOM   7051  CG1 ILE D 435     141.328  10.839  23.519  1.00 39.15      D
ATOM   7052  CD1 ILE D 435     142.476  10.580  22.572  1.00 38.06      D
ATOM   7053  C   ILE D 435     141.273   7.662  25.658  1.00 37.16      D
ATOM   7054  O   ILE D 435     140.130   7.426  26.059  1.00 36.94      D
ATOM   7055  N   LEU D 436     142.360   7.251  26.297  1.00 35.58      D
ATOM   7056  CA  LEU D 436     142.243   6.427  27.481  1.00 34.59      D
ATOM   7057  CB  LEU D 436     142.354   4.980  27.046  1.00 35.11      D
ATOM   7058  CG  LEU D 436     141.894   3.866  27.965  1.00 35.32      D
ATOM   7059  CD1 LEU D 436     142.000   2.560  27.178  1.00 34.07      D
ATOM   7060  CD2 LEU D 436     142.727   3.819  29.234  1.00 35.01      D
ATOM   7061  C   LEU D 436     143.309   6.742  28.511  1.00 34.64      D
ATOM   7062  O   LEU D 436     144.495   6.786  28.195  1.00 35.84      D
ATOM   7063  N   VAL D 437     142.891   6.960  29.750  1.00 33.63      D
ATOM   7064  CA  VAL D 437     143.854   7.244  30.801  1.00 32.09      D
ATOM   7065  CB  VAL D 437     143.484   8.519  31.575  1.00 31.66      D
ATOM   7066  CG1 VAL D 437     144.624   8.902  32.506  1.00 32.49      D
ATOM   7067  CG2 VAL D 437     143.172   9.650  30.608  1.00 31.31      D
ATOM   7068  C   VAL D 437     143.887   6.058  31.764  1.00 31.94      D
ATOM   7069  O   VAL D 437     142.845   5.454  32.047  1.00 31.55      D
ATOM   7070  N   SER D 438     145.080   5.707  32.246  1.00 29.85      D
ATOM   7071  CA  SER D 438     145.201   4.597  33.189  1.00 26.33      D
```

```
ATOM   7072  CB  SER D 438     145.601   3.302  32.480  1.00 25.65      D
ATOM   7073  OG  SER D 438     146.858   3.426  31.852  1.00 26.66      D
ATOM   7074  C   SER D 438     146.156   4.853  34.336  1.00 23.90      D
ATOM   7075  O   SER D 438     146.977   5.765  34.294  1.00 21.89      D
ATOM   7076  N   GLY D 439     146.019   4.025  35.366  1.00 23.29      D
ATOM   7077  CA  GLY D 439     146.835   4.130  36.563  1.00 23.55      D
ATOM   7078  C   GLY D 439     147.396   2.783  36.962  1.00 23.12      D
ATOM   7079  O   GLY D 439     146.725   1.748  36.883  1.00 22.22      D
ATOM   7080  N   SER D 440     148.634   2.800  37.429  1.00 23.85      D
ATOM   7081  CA  SER D 440     149.302   1.562  37.786  1.00 25.71      D
ATOM   7082  CB  SER D 440     150.244   1.169  36.630  1.00 24.70      D
ATOM   7083  OG  SER D 440     151.145   0.129  36.979  1.00 23.47      D
ATOM   7084  C   SER D 440     150.078   1.620  39.099  1.00 26.18      D
ATOM   7085  O   SER D 440     150.112   2.651  39.793  1.00 26.21      D
ATOM   7086  N   THR D 441     150.695   0.481  39.413  1.00 27.38      D
ATOM   7087  CA  THR D 441     151.521   0.308  40.593  1.00 27.39      D
ATOM   7088  CB  THR D 441     151.676  -1.165  40.968  1.00 28.12      D
ATOM   7089  OG1 THR D 441     152.519  -1.810  40.004  1.00 27.63      D
ATOM   7090  CG2 THR D 441     150.310  -1.858  41.003  1.00 28.73      D
ATOM   7091  C   THR D 441     152.903   0.847  40.237  1.00 28.31      D
ATOM   7092  O   THR D 441     153.768   0.906  41.090  1.00 29.00      D
ATOM   7093  N   ASP D 442     153.116   1.234  38.980  1.00 29.46      D
ATOM   7094  CA  ASP D 442     154.402   1.796  38.603  1.00 31.38      D
ATOM   7095  CB  ASP D 442     154.724   1.551  37.126  1.00 33.65      D
ATOM   7096  CG  ASP D 442     153.695   2.167  36.185  1.00 35.87      D
ATOM   7097  OD1 ASP D 442     152.845   2.962  36.680  1.00 35.07      D
ATOM   7098  OD2 ASP D 442     153.753   1.860  34.959  1.00 34.85      D
ATOM   7099  C   ASP D 442     154.351   3.287  38.857  1.00 31.58      D
ATOM   7100  O   ASP D 442     155.161   4.049  38.334  1.00 31.31      D
ATOM   7101  N   ARG D 443     153.360   3.700  39.635  1.00 31.79      D
ATOM   7102  CA  ARG D 443     153.191   5.100  39.983  1.00 31.82      D
ATOM   7103  CB  ARG D 443     154.413   5.569  40.760  1.00 28.96      D
ATOM   7104  CG  ARG D 443     154.805   4.604  41.846  1.00 26.68      D
ATOM   7105  CD  ARG D 443     156.056   5.065  42.541  1.00 25.25      D
ATOM   7106  NE  ARG D 443     156.496   4.111  43.541  1.00 26.33      D
ATOM   7107  CZ  ARG D 443     157.552   4.303  44.319  1.00 27.22      D
ATOM   7108  NH1 ARG D 443     158.250   5.419  44.192  1.00 28.58      D
ATOM   7109  NH2 ARG D 443     157.916   3.388  45.213  1.00 26.32      D
ATOM   7110  C   ARG D 443     152.955   6.016  38.783  1.00 32.05      D
ATOM   7111  O   ARG D 443     152.975   7.243  38.917  1.00 32.48      D
ATOM   7112  N   THR D 444     152.705   5.439  37.616  1.00 31.82      D
ATOM   7113  CA  THR D 444     152.486   6.283  36.459  1.00 32.99      D
ATOM   7114  CB  THR D 444     153.335   5.824  35.246  1.00 32.98      D
ATOM   7115  OG1 THR D 444     152.768   4.643  34.657  1.00 30.88      D
ATOM   7116  CG2 THR D 444     154.757   5.549  35.680  1.00 31.91      D
ATOM   7117  C   THR D 444     151.036   6.451  36.000  1.00 34.38      D
ATOM   7118  O   THR D 444     150.182   5.570  36.164  1.00 34.02      D
ATOM   7119  N   VAL D 445     150.784   7.623  35.432  1.00 35.02      D
ATOM   7120  CA  VAL D 445     149.492   7.992  34.888  1.00 35.88      D
ATOM   7121  CB  VAL D 445     149.049   9.384  35.406  1.00 34.38      D
ATOM   7122  CG1 VAL D 445     147.839   9.871  34.640  1.00 33.91      D
ATOM   7123  CG2 VAL D 445     148.747   9.312  36.893  1.00 33.31      D
ATOM   7124  C   VAL D 445     149.787   8.067  33.392  1.00 38.00      D
ATOM   7125  O   VAL D 445     150.648   8.841  32.969  1.00 40.09      D
```

```
ATOM   7126  N   ARG D 446     149.116   7.256  32.583  1.00 38.70      D
ATOM   7127  CA  ARG D 446     149.390   7.299  31.152  1.00 40.25      D
ATOM   7128  CB  ARG D 446     150.102   6.016  30.707  1.00 40.97      D
ATOM   7129  CG  ARG D 446     151.387   5.796  31.448  1.00 42.38      D
ATOM   7130  CD  ARG D 446     152.190   4.636  30.925  1.00 44.42      D
ATOM   7131  NE  ARG D 446     153.302   4.360  31.835  1.00 48.85      D
ATOM   7132  CZ  ARG D 446     154.291   3.506  31.588  1.00 50.95      D
ATOM   7133  NH1 ARG D 446     154.316   2.834  30.442  1.00 52.13      D
ATOM   7134  NH2 ARG D 446     155.251   3.320  32.490  1.00 51.46      D
ATOM   7135  C   ARG D 446     148.155   7.527  30.296  1.00 40.71      D
ATOM   7136  O   ARG D 446     147.050   7.083  30.635  1.00 39.57      D
ATOM   7137  N   VAL D 447     148.357   8.253  29.195  1.00 40.90      D
ATOM   7138  CA  VAL D 447     147.293   8.552  28.237  1.00 41.54      D
ATOM   7139  CB  VAL D 447     147.260  10.037  27.849  1.00 40.47      D
ATOM   7140  CG1 VAL D 447     146.043  10.306  26.981  1.00 38.69      D
ATOM   7141  CG2 VAL D 447     147.226  10.895  29.100  1.00 40.93      D
ATOM   7142  C   VAL D 447     147.566   7.735  26.991  1.00 42.31      D
ATOM   7143  O   VAL D 447     148.689   7.712  26.501  1.00 43.98      D
ATOM   7144  N   TRP D 448     146.549   7.055  26.481  1.00 42.01      D
ATOM   7145  CA  TRP D 448     146.730   6.234  25.296  1.00 42.06      D
ATOM   7146  CB  TRP D 448     146.416   4.769  25.625  1.00 40.93      D
ATOM   7147  CG  TRP D 448     147.108   4.254  26.849  1.00 40.06      D
ATOM   7148  CD2 TRP D 448     148.167   3.294  26.890  1.00 39.39      D
ATOM   7149  CE2 TRP D 448     148.529   3.127  28.247  1.00 39.74      D
ATOM   7150  CE3 TRP D 448     148.846   2.555  25.911  1.00 37.93      D
ATOM   7151  CD1 TRP D 448     146.871   4.621  28.145  1.00 39.85      D
ATOM   7152  NE1 TRP D 448     147.720   3.949  28.992  1.00 39.87      D
ATOM   7153  CZ2 TRP D 448     149.552   2.247  28.653  1.00 38.84      D
ATOM   7154  CZ3 TRP D 448     149.860   1.680  26.314  1.00 38.08      D
ATOM   7155  CH2 TRP D 448     150.203   1.537  27.679  1.00 37.48      D
ATOM   7156  C   TRP D 448     145.825   6.705  24.156  1.00 42.74      D
ATOM   7157  O   TRP D 448     144.933   7.537  24.349  1.00 42.62      D
ATOM   7158  N   ASP D 449     146.067   6.165  22.967  1.00 43.66      D
ATOM   7159  CA  ASP D 449     145.265   6.485  21.797  1.00 44.36      D
ATOM   7160  CB  ASP D 449     146.062   7.368  20.836  1.00 45.33      D
ATOM   7161  CG  ASP D 449     145.256   7.782  19.616  1.00 46.25      D
ATOM   7162  OD1 ASP D 449     145.791   8.522  18.771  1.00 46.26      D
ATOM   7163  OD2 ASP D 449     144.088   7.370  19.494  1.00 47.22      D
ATOM   7164  C   ASP D 449     144.899   5.169  21.119  1.00 44.82      D
ATOM   7165  O   ASP D 449     145.735   4.551  20.468  1.00 44.81      D
ATOM   7166  N   ILE D 450     143.653   4.740  21.280  1.00 45.73      D
ATOM   7167  CA  ILE D 450     143.205   3.484  20.687  1.00 47.64      D
ATOM   7168  CB  ILE D 450     141.711   3.215  21.000  1.00 46.91      D
ATOM   7169  CG2 ILE D 450     141.335   1.820  20.527  1.00 45.80      D
ATOM   7170  CG1 ILE D 450     141.455   3.357  22.507  1.00 46.32      D
ATOM   7171  CD1 ILE D 450     140.009   3.138  22.920  1.00 46.07      D
ATOM   7172  C   ILE D 450     143.395   3.516  19.173  1.00 49.71      D
ATOM   7173  O   ILE D 450     143.890   2.556  18.573  1.00 49.74      D
ATOM   7174  N   LYS D 451     142.984   4.631  18.571  1.00 51.95      D
ATOM   7175  CA  LYS D 451     143.092   4.859  17.130  1.00 52.66      D
ATOM   7176  CB  LYS D 451     142.789   6.329  16.815  1.00 54.03      D
ATOM   7177  CG  LYS D 451     141.425   6.825  17.283  1.00 54.77      D
ATOM   7178  CD  LYS D 451     140.315   6.348  16.362  1.00 56.08      D
ATOM   7179  CE  LYS D 451     138.958   6.853  16.829  1.00 58.40      D
```

	ATOM	7180	NZ	LYS	D	451	138.564	6.293	18.170	1.00	60.81	D
	ATOM	7181	C	LYS	D	451	144.519	4.534	16.687	1.00	53.12	D
	ATOM	7182	O	LYS	D	451	144.743	3.637	15.875	1.00	52.92	D
	ATOM	7183	N	LYS	D	452	145.478	5.279	17.236	1.00	53.06	D
5	ATOM	7184	CA	LYS	D	452	146.889	5.081	16.922	1.00	53.16	D
	ATOM	7185	CB	LYS	D	452	147.727	6.274	17.405	1.00	54.65	D
	ATOM	7186	CG	LYS	D	452	147.432	7.608	16.705	1.00	55.78	D
	ATOM	7187	CD	LYS	D	452	148.434	8.689	17.106	1.00	54.91	D
	ATOM	7188	CE	LYS	D	452	148.269	9.952	16.262	1.00	56.24	D
10	ATOM	7189	NZ	LYS	D	452	146.931	10.592	16.394	1.00	55.58	D
	ATOM	7190	C	LYS	D	452	147.426	3.801	17.565	1.00	52.16	D
	ATOM	7191	O	LYS	D	452	148.530	3.352	17.257	1.00	52.14	D
	ATOM	7192	N	GLY	D	453	146.646	3.221	18.466	1.00	51.03	D
	ATOM	7193	CA	GLY	D	453	147.070	2.000	19.119	1.00	48.98	D
15	ATOM	7194	C	GLY	D	453	148.425	2.076	19.795	1.00	47.55	D
	ATOM	7195	O	GLY	D	453	149.268	1.206	19.598	1.00	48.41	D
	ATOM	7196	N	CYS	D	454	148.643	3.111	20.595	1.00	45.89	D
	ATOM	7197	CA	CYS	D	454	149.903	3.252	21.306	1.00	45.10	D
	ATOM	7198	CB	CYS	D	454	151.007	3.764	20.371	1.00	45.35	D
20	ATOM	7199	SG	CYS	D	454	151.016	5.592	20.180	1.00	46.05	D
	ATOM	7200	C	CYS	D	454	149.733	4.246	22.445	1.00	45.09	D
	ATOM	7201	O	CYS	D	454	148.660	4.827	22.632	1.00	43.95	D
	ATOM	7202	N	CYS	D	455	150.815	4.443	23.191	1.00	45.72	D
	ATOM	7203	CA	CYS	D	455	150.831	5.373	24.307	1.00	46.22	D
25	ATOM	7204	CB	CYS	D	455	151.663	4.818	25.461	1.00	46.14	D
	ATOM	7205	SG	CYS	D	455	151.652	5.917	26.902	1.00	44.91	D
	ATOM	7206	C	CYS	D	455	151.412	6.717	23.880	1.00	45.90	D
	ATOM	7207	O	CYS	D	455	152.504	6.787	23.328	1.00	45.72	D
	ATOM	7208	N	THR	D	456	150.674	7.778	24.160	1.00	46.41	D
30	ATOM	7209	CA	THR	D	456	151.089	9.114	23.807	1.00	47.30	D
	ATOM	7210	CB	THR	D	456	149.878	9.947	23.316	1.00	47.67	D
	ATOM	7211	OG1	THR	D	456	150.170	11.344	23.454	1.00	49.91	D
	ATOM	7212	CG2	THR	D	456	148.633	9.623	24.124	1.00	48.32	D
	ATOM	7213	C	THR	D	456	151.767	9.870	24.953	1.00	47.34	D
35	ATOM	7214	O	THR	D	456	152.722	10.614	24.729	1.00	47.57	D
	ATOM	7215	N	HIS	D	457	151.280	9.691	26.177	1.00	46.90	D
	ATOM	7216	CA	HIS	D	457	151.850	10.407	27.315	1.00	46.66	D
	ATOM	7217	CB	HIS	D	457	150.935	11.569	27.708	1.00	48.78	D
	ATOM	7218	CG	HIS	D	457	150.781	12.608	26.639	1.00	52.07	D
40	ATOM	7219	CD2	HIS	D	457	149.752	12.884	25.802	1.00	53.00	D
	ATOM	7220	ND1	HIS	D	457	151.768	13.525	26.349	1.00	51.90	D
	ATOM	7221	CE1	HIS	D	457	151.351	14.324	25.383	1.00	53.55	D
	ATOM	7222	NE2	HIS	D	457	150.131	13.957	25.033	1.00	53.69	D
	ATOM	7223	C	HIS	D	457	152.101	9.534	28.529	1.00	45.09	D
45	ATOM	7224	O	HIS	D	457	151.360	8.591	28.797	1.00	46.21	D
	ATOM	7225	N	VAL	D	458	153.163	9.864	29.255	1.00	43.08	D
	ATOM	7226	CA	VAL	D	458	153.544	9.142	30.462	1.00	40.12	D
	ATOM	7227	CB	VAL	D	458	154.847	8.350	30.247	1.00	38.48	D
	ATOM	7228	CG1	VAL	D	458	155.106	7.437	31.430	1.00	36.35	D
50	ATOM	7229	CG2	VAL	D	458	154.758	7.554	28.954	1.00	37.80	D
	ATOM	7230	C	VAL	D	458	153.761	10.197	31.535	1.00	38.68	D
	ATOM	7231	O	VAL	D	458	154.733	10.942	31.474	1.00	38.06	D
	ATOM	7232	N	PHE	D	459	152.834	10.267	32.491	1.00	37.03	D
	ATOM	7233	CA	PHE	D	459	152.902	11.230	33.588	1.00	35.98	D

```
ATOM   7234  CB  PHE D 459     151.526  11.848  33.859  1.00 35.38      D
ATOM   7235  CG  PHE D 459     151.009  12.705  32.729  1.00 36.52      D
ATOM   7236  CD1 PHE D 459     149.643  12.975  32.603  1.00 35.53      D
ATOM   7237  CD2 PHE D 459     151.882  13.228  31.773  1.00 36.02      D
ATOM   7238  CE1 PHE D 459     149.160  13.748  31.542  1.00 33.32      D
ATOM   7239  CE2 PHE D 459     151.404  13.999  30.715  1.00 34.61      D
ATOM   7240  CZ  PHE D 459     150.040  14.258  30.599  1.00 33.14      D
ATOM   7241  C   PHE D 459     153.421  10.583  34.858  1.00 35.63      D
ATOM   7242  O   PHE D 459     152.927   9.540  35.286  1.00 36.76      D
ATOM   7243  N   GLU D 460     154.436  11.210  35.443  1.00 34.40      D
ATOM   7244  CA  GLU D 460     155.042  10.731  36.669  1.00 32.85      D
ATOM   7245  CB  GLU D 460     156.541  10.572  36.501  1.00 31.50      D
ATOM   7246  CG  GLU D 460     156.912   9.591  35.436  1.00 34.06      D
ATOM   7247  CD  GLU D 460     158.340   9.146  35.561  1.00 34.99      D
ATOM   7248  OE1 GLU D 460     159.177   9.996  35.916  1.00 38.06      D
ATOM   7249  OE2 GLU D 460     158.634   7.959  35.305  1.00 34.49      D
ATOM   7250  C   GLU D 460     154.754  11.770  37.717  1.00 32.81      D
ATOM   7251  O   GLU D 460     154.506  12.927  37.387  1.00 33.34      D
ATOM   7252  N   GLY D 461     154.788  11.364  38.982  1.00 33.03      D
ATOM   7253  CA  GLY D 461     154.503  12.295  40.057  1.00 31.23      D
ATOM   7254  C   GLY D 461     154.150  11.600  41.354  1.00 30.79      D
ATOM   7255  O   GLY D 461     154.770  11.857  42.383  1.00 31.55      D
ATOM   7256  N   HIS D 462     153.151  10.727  41.318  1.00 30.63      D
ATOM   7257  CA  HIS D 462     152.744  10.016  42.522  1.00 30.77      D
ATOM   7258  CB  HIS D 462     151.580   9.065  42.209  1.00 30.12      D
ATOM   7259  CG  HIS D 462     150.254   9.754  42.066  1.00 29.59      D
ATOM   7260  CD2 HIS D 462     149.387   9.814  41.026  1.00 29.20      D
ATOM   7261  ND1 HIS D 462     149.701  10.520  43.070  1.00 27.98      D
ATOM   7262  CE1 HIS D 462     148.555  11.027  42.652  1.00 29.48      D
ATOM   7263  NE2 HIS D 462     148.342  10.615  41.415  1.00 29.45      D
ATOM   7264  C   HIS D 462     153.935   9.233  43.032  1.00 31.13      D
ATOM   7265  O   HIS D 462     154.687   8.672  42.240  1.00 32.76      D
ATOM   7266  N   ASN D 463     154.113   9.195  44.349  1.00 31.08      D
ATOM   7267  CA  ASN D 463     155.239   8.473  44.929  1.00 30.79      D
ATOM   7268  CB  ASN D 463     155.764   9.212  46.155  1.00 31.33      D
ATOM   7269  CG  ASN D 463     156.351  10.572  45.806  1.00 33.80      D
ATOM   7270  OD1 ASN D 463     156.669  11.368  46.700  1.00 36.56      D
ATOM   7271  ND2 ASN D 463     156.500  10.848  44.511  1.00 31.92      D
ATOM   7272  C   ASN D 463     154.863   7.058  45.300  1.00 30.83      D
ATOM   7273  O   ASN D 463     155.678   6.319  45.843  1.00 32.01      D
ATOM   7274  N   SER D 464     153.623   6.685  44.996  1.00 30.09      D
ATOM   7275  CA  SER D 464     153.099   5.346  45.292  1.00 29.60      D
ATOM   7276  CB  SER D 464     152.364   5.358  46.630  1.00 31.07      D
ATOM   7277  OG  SER D 464     153.073   4.621  47.611  1.00 34.87      D
ATOM   7278  C   SER D 464     152.125   4.900  44.203  1.00 28.55      D
ATOM   7279  O   SER D 464     151.814   5.656  43.289  1.00 29.29      D
ATOM   7280  N   THR D 465     151.625   3.676  44.313  1.00 27.12      D
ATOM   7281  CA  THR D 465     150.675   3.153  43.331  1.00 25.67      D
ATOM   7282  CB  THR D 465     150.036   1.828  43.817  1.00 23.85      D
ATOM   7283  OG1 THR D 465     151.057   0.894  44.197  1.00 24.69      D
ATOM   7284  CG2 THR D 465     149.169   1.234  42.742  1.00 22.12      D
ATOM   7285  C   THR D 465     149.536   4.150  43.089  1.00 26.17      D
ATOM   7286  O   THR D 465     149.122   4.872  44.001  1.00 27.21      D
ATOM   7287  N   VAL D 466     149.041   4.197  41.856  1.00 25.63      D
```

```
ATOM   7288  CA  VAL D 466     147.933   5.078  41.506  1.00 24.45      D
ATOM   7289  CB  VAL D 466     148.003   5.484  39.994  1.00 26.90      D
ATOM   7290  CG1 VAL D 466     146.795   6.351  39.597  1.00 27.11      D
ATOM   7291  CG2 VAL D 466     149.300   6.240  39.732  1.00 27.75      D
ATOM   7292  C   VAL D 466     146.740   4.165  41.783  1.00 22.49      D
ATOM   7293  O   VAL D 466     146.604   3.130  41.148  1.00 19.72      D
ATOM   7294  N   ARG D 467     145.894   4.543  42.737  1.00 21.80      D
ATOM   7295  CA  ARG D 467     144.764   3.713  43.121  1.00 21.09      D
ATOM   7296  CB  ARG D 467     144.529   3.828  44.637  1.00 21.63      D
ATOM   7297  CG  ARG D 467     143.582   2.778  45.221  1.00 24.03      D
ATOM   7298  CD  ARG D 467     144.190   1.398  45.033  1.00 25.89      D
ATOM   7299  NE  ARG D 467     143.247   0.294  45.158  1.00 27.91      D
ATOM   7300  CZ  ARG D 467     142.283   0.013  44.288  1.00 30.10      D
ATOM   7301  NH1 ARG D 467     142.117   0.776  43.214  1.00 32.22      D
ATOM   7302  NH2 ARG D 467     141.515  -1.064  44.469  1.00 28.51      D
ATOM   7303  C   ARG D 467     143.463   3.984  42.370  1.00 21.53      D
ATOM   7304  O   ARG D 467     142.666   3.071  42.152  1.00 21.18      D
ATOM   7305  N   CYS D 468     143.240   5.225  41.960  1.00 21.08      D
ATOM   7306  CA  CYS D 468     142.008   5.538  41.259  1.00 22.04      D
ATOM   7307  CB  CYS D 468     140.874   5.672  42.282  1.00 22.73      D
ATOM   7308  SG  CYS D 468     141.036   7.052  43.480  1.00 26.78      D
ATOM   7309  C   CYS D 468     142.141   6.807  40.433  1.00 22.89      D
ATOM   7310  O   CYS D 468     143.034   7.617  40.672  1.00 24.06      D
ATOM   7311  N   LEU D 469     141.247   6.995  39.466  1.00 23.65      D
ATOM   7312  CA  LEU D 469     141.321   8.189  38.614  1.00 25.22      D
ATOM   7313  CB  LEU D 469     142.382   7.997  37.512  1.00 25.67      D
ATOM   7314  CG  LEU D 469     142.191   6.914  36.441  1.00 25.46      D
ATOM   7315  CD1 LEU D 469     140.965   7.170  35.605  1.00 24.47      D
ATOM   7316  CD2 LEU D 469     143.428   6.891  35.560  1.00 26.81      D
ATOM   7317  C   LEU D 469     140.005   8.574  37.960  1.00 24.60      D
ATOM   7318  O   LEU D 469     139.162   7.729  37.690  1.00 24.12      D
ATOM   7319  N   ASP D 470     139.818   9.853  37.693  1.00 24.30      D
ATOM   7320  CA  ASP D 470     138.584  10.242  37.043  1.00 24.73      D
ATOM   7321  CB  ASP D 470     137.540  10.594  38.118  1.00 24.80      D
ATOM   7322  CG  ASP D 470     136.109  10.685  37.571  1.00 24.84      D
ATOM   7323  OD1 ASP D 470     135.842  10.240  36.441  1.00 25.89      D
ATOM   7324  OD2 ASP D 470     135.242  11.197  38.296  1.00 23.60      D
ATOM   7325  C   ASP D 470     138.857  11.409  36.091  1.00 24.57      D
ATOM   7326  O   ASP D 470     139.863  12.118  36.214  1.00 23.14      D
ATOM   7327  N   ILE D 471     137.988  11.584  35.110  1.00 24.45      D
ATOM   7328  CA  ILE D 471     138.184  12.684  34.197  1.00 26.31      D
ATOM   7329  CB  ILE D 471     138.389  12.210  32.737  1.00 24.06      D
ATOM   7330  CG2 ILE D 471     138.861  13.393  31.915  1.00 24.13      D
ATOM   7331  CG1 ILE D 471     139.454  11.097  32.656  1.00 22.43      D
ATOM   7332  CD1 ILE D 471     139.553  10.449  31.293  1.00 18.18      D
ATOM   7333  C   ILE D 471     136.971  13.600  34.271  1.00 28.56      D
ATOM   7334  O   ILE D 471     135.833  13.135  34.280  1.00 30.74      D
ATOM   7335  N   VAL D 472     137.222  14.901  34.358  1.00 30.47      D
ATOM   7336  CA  VAL D 472     136.157  15.892  34.433  1.00 31.86      D
ATOM   7337  CB  VAL D 472     136.105  16.544  35.857  1.00 31.83      D
ATOM   7338  CG1 VAL D 472     135.793  15.474  36.896  1.00 30.28      D
ATOM   7339  CG2 VAL D 472     137.427  17.231  36.193  1.00 27.41      D
ATOM   7340  C   VAL D 472     136.369  16.966  33.358  1.00 33.87      D
ATOM   7341  O   VAL D 472     137.474  17.119  32.826  1.00 34.57      D
```

```
ATOM   7342  N   GLU D 473     135.304  17.692  33.026  1.00 35.69      D
ATOM   7343  CA  GLU D 473     135.354  18.747  32.004  1.00 37.97      D
ATOM   7344  CB  GLU D 473     134.565  18.321  30.751  1.00 39.26      D
ATOM   7345  CG  GLU D 473     134.587  19.326  29.567  1.00 41.82      D
ATOM   7346  CD  GLU D 473     133.581  18.966  28.455  1.00 41.92      D
ATOM   7347  OE1 GLU D 473     133.651  17.853  27.893  1.00 41.68      D
ATOM   7348  OE2 GLU D 473     132.712  19.801  28.145  1.00 42.75      D
ATOM   7349  C   GLU D 473     134.722  19.983  32.620  1.00 38.63      D
ATOM   7350  O   GLU D 473     133.585  19.944  33.084  1.00 39.66      D
ATOM   7351  N   TYR D 474     135.464  21.077  32.651  1.00 39.16      D
ATOM   7352  CA  TYR D 474     134.952  22.311  33.231  1.00 39.98      D
ATOM   7353  CB  TYR D 474     135.534  22.496  34.630  1.00 39.54      D
ATOM   7354  CG  TYR D 474     135.126  23.777  35.311  1.00 40.62      D
ATOM   7355  CD1 TYR D 474     133.802  24.002  35.686  1.00 40.93      D
ATOM   7356  CE1 TYR D 474     133.432  25.174  36.332  1.00 40.40      D
ATOM   7357  CD2 TYR D 474     136.072  24.761  35.601  1.00 40.52      D
ATOM   7358  CE2 TYR D 474     135.714  25.933  36.243  1.00 40.34      D
ATOM   7359  CZ  TYR D 474     134.393  26.134  36.604  1.00 40.71      D
ATOM   7360  OH  TYR D 474     134.025  27.300  37.224  1.00 41.79      D
ATOM   7361  C   TYR D 474     135.422  23.394  32.277  1.00 39.99      D
ATOM   7362  O   TYR D 474     136.550  23.339  31.784  1.00 40.02      D
ATOM   7363  N   LYS D 475     134.551  24.357  31.998  1.00 40.09      D
ATOM   7364  CA  LYS D 475     134.868  25.438  31.069  1.00 42.55      D
ATOM   7365  CB  LYS D 475     135.796  26.471  31.723  1.00 43.10      D
ATOM   7366  CG  LYS D 475     135.185  27.292  32.864  1.00 43.55      D
ATOM   7367  CD  LYS D 475     136.276  28.148  33.502  1.00 46.85      D
ATOM   7368  CE  LYS D 475     135.765  29.052  34.623  1.00 48.93      D
ATOM   7369  NZ  LYS D 475     134.765  30.077  34.181  1.00 49.55      D
ATOM   7370  C   LYS D 475     135.529  24.888  29.804  1.00 43.23      D
ATOM   7371  O   LYS D 475     136.556  25.401  29.352  1.00 43.08      D
ATOM   7372  N   ASN D 476     134.943  23.831  29.248  1.00 44.27      D
ATOM   7373  CA  ASN D 476     135.449  23.202  28.024  1.00 44.54      D
ATOM   7374  CB  ASN D 476     135.383  24.180  26.850  1.00 44.94      D
ATOM   7375  CG  ASN D 476     134.054  24.135  26.140  1.00 44.85      D
ATOM   7376  OD1 ASN D 476     133.040  24.596  26.665  1.00 44.09      D
ATOM   7377  ND2 ASN D 476     134.048  23.565  24.934  1.00 45.89      D
ATOM   7378  C   ASN D 476     136.841  22.591  28.077  1.00 44.03      D
ATOM   7379  O   ASN D 476     137.403  22.230  27.036  1.00 44.45      D
ATOM   7380  N   ILE D 477     137.400  22.474  29.280  1.00 43.98      D
ATOM   7381  CA  ILE D 477     138.722  21.860  29.459  1.00 42.39      D
ATOM   7382  CB  ILE D 477     139.681  22.744  30.260  1.00 42.82      D
ATOM   7383  CG2 ILE D 477     141.024  22.052  30.387  1.00 43.06      D
ATOM   7384  CG1 ILE D 477     139.842  24.097  29.583  1.00 42.36      D
ATOM   7385  CD1 ILE D 477     140.465  25.135  30.486  1.00 41.94      D
ATOM   7386  C   ILE D 477     138.528  20.578  30.249  1.00 41.19      D
ATOM   7387  O   ILE D 477     137.805  20.560  31.253  1.00 40.43      D
ATOM   7388  N   LYS D 478     139.166  19.511  29.777  1.00 38.84      D
ATOM   7389  CA  LYS D 478     139.078  18.212  30.428  1.00 36.96      D
ATOM   7390  CB  LYS D 478     139.070  17.085  29.394  1.00 35.75      D
ATOM   7391  CG  LYS D 478     137.740  16.932  28.687  1.00 35.23      D
ATOM   7392  CD  LYS D 478     137.557  15.519  28.160  1.00 32.30      D
ATOM   7393  CE  LYS D 478     136.120  15.312  27.725  1.00 31.88      D
ATOM   7394  NZ  LYS D 478     135.743  13.871  27.552  1.00 32.71      D
ATOM   7395  C   LYS D 478     140.218  17.984  31.402  1.00 36.46      D
```

```
ATOM   7396  O   LYS D 478     141.381  18.009  31.015  1.00 36.77      D
ATOM   7397  N   TYR D 479     139.884  17.749  32.666  1.00 35.14      D
ATOM   7398  CA  TYR D 479     140.906  17.514  33.675  1.00 34.37      D
ATOM   7399  CB  TYR D 479     140.674  18.442  34.875  1.00 33.93      D
ATOM   7400  CG  TYR D 479     140.847  19.914  34.543  1.00 34.98      D
ATOM   7401  CD1 TYR D 479     142.108  20.529  34.614  1.00 33.05      D
ATOM   7402  CE1 TYR D 479     142.264  21.880  34.300  1.00 32.76      D
ATOM   7403  CD2 TYR D 479     139.753  20.691  34.147  1.00 33.92      D
ATOM   7404  CE2 TYR D 479     139.901  22.037  33.830  1.00 34.11      D
ATOM   7405  CZ  TYR D 479     141.152  22.624  33.907  1.00 34.22      D
ATOM   7406  OH  TYR D 479     141.270  23.952  33.573  1.00 37.80      D
ATOM   7407  C   TYR D 479     140.936  16.061  34.134  1.00 32.92      D
ATOM   7408  O   TYR D 479     139.903  15.404  34.218  1.00 32.94      D
ATOM   7409  N   ILE D 480     142.138  15.569  34.412  1.00 31.23      D
ATOM   7410  CA  ILE D 480     142.344  14.213  34.910  1.00 30.00      D
ATOM   7411  CB  ILE D 480     143.568  13.528  34.236  1.00 30.27      D
ATOM   7412  CG2 ILE D 480     143.826  12.150  34.879  1.00 31.07      D
ATOM   7413  CG1 ILE D 480     143.335  13.334  32.741  1.00 31.12      D
ATOM   7414  CD1 ILE D 480     144.440  12.531  32.060  1.00 26.66      D
ATOM   7415  C   ILE D 480     142.674  14.314  36.417  1.00 29.96      D
ATOM   7416  O   ILE D 480     143.583  15.063  36.808  1.00 29.34      D
ATOM   7417  N   VAL D 481     141.944  13.582  37.263  1.00 28.07      D
ATOM   7418  CA  VAL D 481     142.234  13.590  38.702  1.00 26.17      D
ATOM   7419  CB  VAL D 481     141.048  14.099  39.550  1.00 25.50      D
ATOM   7420  CG1 VAL D 481     141.533  14.438  40.943  1.00 25.80      D
ATOM   7421  CG2 VAL D 481     140.431  15.338  38.910  1.00 26.04      D
ATOM   7422  C   VAL D 481     142.587  12.166  39.110  1.00 26.07      D
ATOM   7423  O   VAL D 481     141.848  11.232  38.812  1.00 26.50      D
ATOM   7424  N   THR D 482     143.734  12.006  39.766  1.00 26.06      D
ATOM   7425  CA  THR D 482     144.217  10.691  40.184  1.00 26.60      D
ATOM   7426  CB  THR D 482     145.520  10.324  39.440  1.00 25.75      D
ATOM   7427  OG1 THR D 482     146.452  11.402  39.568  1.00 23.78      D
ATOM   7428  CG2 THR D 482     145.252  10.057  37.971  1.00 26.32      D
ATOM   7429  C   THR D 482     144.496  10.591  41.688  1.00 27.46      D
ATOM   7430  O   THR D 482     145.180  11.444  42.267  1.00 29.29      D
ATOM   7431  N   GLY D 483     143.977   9.530  42.303  1.00 25.97      D
ATOM   7432  CA  GLY D 483     144.176   9.303  43.724  1.00 24.32      D
ATOM   7433  C   GLY D 483     145.201   8.206  43.922  1.00 23.49      D
ATOM   7434  O   GLY D 483     145.156   7.171  43.236  1.00 23.98      D
ATOM   7435  N   SER D 484     146.106   8.428  44.877  1.00 22.04      D
ATOM   7436  CA  SER D 484     147.208   7.503  45.153  1.00 21.89      D
ATOM   7437  CB  SER D 484     148.540   8.193  44.820  1.00 19.14      D
ATOM   7438  OG  SER D 484     149.640   7.324  45.038  1.00 17.25      D
ATOM   7439  C   SER D 484     147.266   7.012  46.582  1.00 22.62      D
ATOM   7440  O   SER D 484     146.488   7.433  47.426  1.00 25.82      D
ATOM   7441  N   ARG D 485     148.193   6.100  46.837  1.00 24.32      D
ATOM   7442  CA  ARG D 485     148.412   5.585  48.179  1.00 26.12      D
ATOM   7443  CB  ARG D 485     149.052   4.206  48.134  1.00 27.36      D
ATOM   7444  CG  ARG D 485     148.168   3.160  47.556  1.00 28.76      D
ATOM   7445  CD  ARG D 485     148.786   1.809  47.722  1.00 29.11      D
ATOM   7446  NE  ARG D 485     147.768   0.784  47.543  1.00 31.30      D
ATOM   7447  CZ  ARG D 485     148.031  -0.500  47.350  1.00 31.33      D
ATOM   7448  NH1 ARG D 485     149.283  -0.931  47.304  1.00 30.94      D
ATOM   7449  NH2 ARG D 485     147.039  -1.353  47.214  1.00 31.96      D
```

```
ATOM   7450  C   ARG D 485     149.367   6.534  48.886  1.00 27.46      D
ATOM   7451  O   ARG D 485     149.712   6.329  50.045  1.00 28.74      D
ATOM   7452  N   ASP D 486     149.822   7.561  48.186  1.00 27.88      D
ATOM   7453  CA  ASP D 486     150.722   8.487  48.819  1.00 27.38      D
ATOM   7454  CB  ASP D 486     151.631   9.137  47.789  1.00 29.39      D
ATOM   7455  CG  ASP D 486     150.858   9.822  46.695  1.00 30.30      D
ATOM   7456  OD1 ASP D 486     149.693  10.190  46.951  1.00 28.83      D
ATOM   7457  OD2 ASP D 486     151.410  10.006  45.591  1.00 33.15      D
ATOM   7458  C   ASP D 486     149.947   9.547  49.566  1.00 26.08      D
ATOM   7459  O   ASP D 486     150.524  10.533  49.997  1.00 26.51      D
ATOM   7460  N   ASN D 487     148.643   9.343  49.727  1.00 26.47      D
ATOM   7461  CA  ASN D 487     147.778  10.295  50.449  1.00 28.03      D
ATOM   7462  CB  ASN D 487     148.466  10.859  51.720  1.00 24.22      D
ATOM   7463  CG  ASN D 487     149.130   9.783  52.608  1.00 25.85      D
ATOM   7464  OD1 ASN D 487     150.077  10.094  53.357  1.00 25.75      D
ATOM   7465  ND2 ASN D 487     148.639   8.536  52.543  1.00 23.88      D
ATOM   7466  C   ASN D 487     147.331  11.492  49.578  1.00 29.17      D
ATOM   7467  O   ASN D 487     146.419  12.233  49.958  1.00 30.88      D
ATOM   7468  N   THR D 488     147.959  11.686  48.419  1.00 30.51      D
ATOM   7469  CA  THR D 488     147.599  12.817  47.574  1.00 31.76      D
ATOM   7470  CB  THR D 488     148.867  13.590  47.044  1.00 32.19      D
ATOM   7471  OG1 THR D 488     149.361  12.984  45.841  1.00 30.87      D
ATOM   7472  CG2 THR D 488     149.968  13.586  48.078  1.00 32.86      D
ATOM   7473  C   THR D 488     146.708  12.444  46.387  1.00 33.20      D
ATOM   7474  O   THR D 488     146.374  11.267  46.172  1.00 32.98      D
ATOM   7475  N   LEU D 489     146.310  13.480  45.650  1.00 34.03      D
ATOM   7476  CA  LEU D 489     145.468  13.377  44.465  1.00 34.19      D
ATOM   7477  CB  LEU D 489     144.056  13.869  44.779  1.00 34.15      D
ATOM   7478  CG  LEU D 489     143.138  12.961  45.589  1.00 34.12      D
ATOM   7479  CD1 LEU D 489     142.459  13.747  46.710  1.00 33.50      D
ATOM   7480  CD2 LEU D 489     142.102  12.369  44.642  1.00 32.16      D
ATOM   7481  C   LEU D 489     146.084  14.320  43.448  1.00 33.40      D
ATOM   7482  O   LEU D 489     145.854  15.519  43.533  1.00 34.39      D
ATOM   7483  N   HIS D 490     146.876  13.818  42.506  1.00 32.48      D
ATOM   7484  CA  HIS D 490     147.465  14.727  41.522  1.00 31.60      D
ATOM   7485  CB  HIS D 490     148.744  14.136  40.909  1.00 31.07      D
ATOM   7486  CG  HIS D 490     149.914  14.125  41.846  1.00 31.65      D
ATOM   7487  CD2 HIS D 490     149.977  14.042  43.197  1.00 32.29      D
ATOM   7488  ND1 HIS D 490     151.219  14.191  41.407  1.00 33.73      D
ATOM   7489  CE1 HIS D 490     152.036  14.152  42.446  1.00 33.37      D
ATOM   7490  NE2 HIS D 490     151.306  14.061  43.543  1.00 32.68      D
ATOM   7491  C   HIS D 490     146.456  15.034  40.429  1.00 30.39      D
ATOM   7492  O   HIS D 490     145.735  14.149  39.983  1.00 31.27      D
ATOM   7493  N   VAL D 491     146.391  16.296  40.022  1.00 29.80      D
ATOM   7494  CA  VAL D 491     145.466  16.726  38.977  1.00 31.12      D
ATOM   7495  CB  VAL D 491     144.610  17.941  39.472  1.00 30.67      D
ATOM   7496  CG1 VAL D 491     143.683  18.442  38.365  1.00 29.26      D
ATOM   7497  CG2 VAL D 491     143.798  17.544  40.683  1.00 29.19      D
ATOM   7498  C   VAL D 491     146.256  17.127  37.712  1.00 32.27      D
ATOM   7499  O   VAL D 491     147.249  17.850  37.802  1.00 33.21      D
ATOM   7500  N   TRP D 492     145.829  16.647  36.545  1.00 32.46      D
ATOM   7501  CA  TRP D 492     146.501  16.975  35.285  1.00 33.55      D
ATOM   7502  CB  TRP D 492     147.308  15.798  34.759  1.00 33.18      D
ATOM   7503  CG  TRP D 492     147.697  14.828  35.788  1.00 34.51      D
```

```
ATOM   7504  CD2 TRP D 492     149.014  14.604  36.288  1.00 35.06      D
ATOM   7505  CE2 TRP D 492     148.930  13.552  37.224  1.00 34.88      D
ATOM   7506  CE3 TRP D 492     150.263  15.189  36.034  1.00 33.09      D
ATOM   7507  CD1 TRP D 492     146.884  13.936  36.423  1.00 34.18      D
ATOM   7508  NE1 TRP D 492     147.617  13.161  37.285  1.00 34.58      D
ATOM   7509  CZ2 TRP D 492     150.048  13.073  37.906  1.00 34.36      D
ATOM   7510  CZ3 TRP D 492     151.371  14.715  36.710  1.00 32.50      D
ATOM   7511  CH2 TRP D 492     151.258  13.667  37.634  1.00 33.38      D
ATOM   7512  C   TRP D 492     145.475  17.318  34.226  1.00 34.32      D
ATOM   7513  O   TRP D 492     144.338  16.864  34.292  1.00 35.53      D
ATOM   7514  N   LYS D 493     145.859  18.110  33.236  1.00 34.28      D
ATOM   7515  CA  LYS D 493     144.900  18.433  32.202  1.00 35.06      D
ATOM   7516  CB  LYS D 493     145.116  19.860  31.694  1.00 35.38      D
ATOM   7517  CG  LYS D 493     146.531  20.133  31.281  1.00 37.78      D
ATOM   7518  CD  LYS D 493     146.739  21.563  30.810  1.00 39.13      D
ATOM   7519  CE  LYS D 493     146.643  22.588  31.928  1.00 37.56      D
ATOM   7520  NZ  LYS D 493     147.094  23.906  31.410  1.00 35.80      D
ATOM   7521  C   LYS D 493     145.075  17.408  31.084  1.00 34.97      D
ATOM   7522  O   LYS D 493     146.182  17.192  30.600  1.00 33.77      D
ATOM   7523  N   LEU D 494     143.981  16.753  30.706  1.00 36.70      D
ATOM   7524  CA  LEU D 494     144.018  15.744  29.659  1.00 39.45      D
ATOM   7525  CB  LEU D 494     142.630  15.126  29.458  1.00 39.18      D
ATOM   7526  CG  LEU D 494     142.458  14.046  28.380  1.00 38.09      D
ATOM   7527  CD1 LEU D 494     143.506  12.972  28.552  1.00 36.77      D
ATOM   7528  CD2 LEU D 494     141.043  13.442  28.448  1.00 36.96      D
ATOM   7529  C   LEU D 494     144.493  16.382  28.366  1.00 42.52      D
ATOM   7530  O   LEU D 494     143.928  17.387  27.912  1.00 42.98      D
ATOM   7531  N   PRO D 495     145.559  15.819  27.764  1.00 45.09      D
ATOM   7532  CD  PRO D 495     146.315  14.686  28.330  1.00 45.01      D
ATOM   7533  CA  PRO D 495     146.168  16.287  26.505  1.00 45.59      D
ATOM   7534  CB  PRO D 495     147.255  15.253  26.241  1.00 45.10      D
ATOM   7535  CG  PRO D 495     147.633  14.802  27.619  1.00 45.87      D
ATOM   7536  C   PRO D 495     145.146  16.324  25.365  1.00 46.50      D
ATOM   7537  O   PRO D 495     144.334  15.409  25.243  1.00 47.18      D
ATOM   7538  N   LYS D 496     145.194  17.360  24.525  1.00 47.14      D
ATOM   7539  CA  LYS D 496     144.254  17.491  23.400  1.00 47.35      D
ATOM   7540  CB  LYS D 496     143.768  18.942  23.268  1.00 47.30      D
ATOM   7541  CG  LYS D 496     143.109  19.501  24.520  0.00 47.88      D
ATOM   7542  CD  LYS D 496     141.811  18.778  24.840  0.00 48.23      D
ATOM   7543  CE  LYS D 496     141.133  19.370  26.065  0.00 48.50      D
ATOM   7544  NZ  LYS D 496     139.817  18.722  26.331  0.00 48.74      D
ATOM   7545  C   LYS D 496     144.853  17.046  22.064  1.00 47.41      D
ATOM   7546  O   LYS D 496     145.277  15.898  21.895  1.00 46.92      D
ATOM   7547  N   ASP D 508     157.546   8.144  18.136  1.00 82.08      D
ATOM   7548  CA  ASP D 508     158.190   8.937  19.182  1.00 81.66      D
ATOM   7549  CB  ASP D 508     158.981  10.090  18.569  1.00 82.86      D
ATOM   7550  CG  ASP D 508     158.086  11.249  18.168  1.00 83.90      D
ATOM   7551  OD1 ASP D 508     157.135  11.025  17.381  1.00 83.92      D
ATOM   7552  OD2 ASP D 508     158.334  12.378  18.644  1.00 83.63      D
ATOM   7553  C   ASP D 508     157.121   9.528  20.096  1.00 80.44      D
ATOM   7554  O   ASP D 508     157.419  10.346  20.972  1.00 80.05      D
ATOM   7555  N   TYR D 509     155.874   9.120  19.884  1.00 78.72      D
ATOM   7556  CA  TYR D 509     154.768   9.631  20.678  1.00 76.03      D
ATOM   7557  CB  TYR D 509     153.454   8.997  20.254  1.00 76.05      D
```

```
ATOM   7558  CG  TYR D 509     152.443  10.025  19.841  1.00 77.13      D
ATOM   7559  CD1 TYR D 509     152.268  11.195  20.579  1.00 77.84      D
ATOM   7560  CE1 TYR D 509     151.324  12.147  20.205  1.00 79.73      D
ATOM   7561  CD2 TYR D 509     151.653   9.830  18.719  1.00 78.10      D
ATOM   7562  CE2 TYR D 509     150.709  10.769  18.335  1.00 79.97      D
ATOM   7563  CZ  TYR D 509     150.543  11.923  19.080  1.00 80.67      D
ATOM   7564  OH  TYR D 509     149.570  12.832  18.715  1.00 82.17      D
ATOM   7565  C   TYR D 509     154.938   9.440  22.170  1.00 73.80      D
ATOM   7566  O   TYR D 509     154.457  10.253  22.960  1.00 75.57      D
ATOM   7567  N   PRO D 510     155.602   8.352  22.588  1.00 70.29      D
ATOM   7568  CD  PRO D 510     156.084   7.160  21.860  1.00 68.38      D
ATOM   7569  CA  PRO D 510     155.758   8.194  24.039  1.00 66.01      D
ATOM   7570  CB  PRO D 510     156.600   6.929  24.150  1.00 66.48      D
ATOM   7571  CG  PRO D 510     156.132   6.128  22.949  1.00 68.27      D
ATOM   7572  C   PRO D 510     156.446   9.424  24.644  1.00 62.34      D
ATOM   7573  O   PRO D 510     157.667   9.504  24.676  1.00 62.17      D
ATOM   7574  N   LEU D 511     155.655  10.392  25.096  1.00 58.50      D
ATOM   7575  CA  LEU D 511     156.197  11.603  25.700  1.00 54.92      D
ATOM   7576  CB  LEU D 511     155.354  12.806  25.313  1.00 54.10      D
ATOM   7577  CG  LEU D 511     155.130  12.940  23.807  1.00 52.83      D
ATOM   7578  CD1 LEU D 511     154.228  14.114  23.521  1.00 51.33      D
ATOM   7579  CD2 LEU D 511     156.467  13.102  23.107  1.00 52.54      D
ATOM   7580  C   LEU D 511     156.188  11.451  27.211  1.00 53.49      D
ATOM   7581  O   LEU D 511     155.145  11.576  27.847  1.00 53.00      D
ATOM   7582  N   VAL D 512     157.359  11.184  27.778  1.00 52.14      D
ATOM   7583  CA  VAL D 512     157.506  10.992  29.213  1.00 49.88      D
ATOM   7584  CB  VAL D 512     158.576   9.937  29.498  1.00 48.71      D
ATOM   7585  CG1 VAL D 512     158.654   9.664  30.992  1.00 49.81      D
ATOM   7586  CG2 VAL D 512     158.262   8.666  28.725  1.00 47.64      D
ATOM   7587  C   VAL D 512     157.889  12.265  29.954  1.00 49.28      D
ATOM   7588  O   VAL D 512     158.855  12.925  29.592  1.00 48.19      D
ATOM   7589  N   PHE D 513     157.126  12.598  30.994  1.00 50.24      D
ATOM   7590  CA  PHE D 513     157.397  13.778  31.823  1.00 51.82      D
ATOM   7591  CB  PHE D 513     156.158  14.671  31.950  1.00 51.83      D
ATOM   7592  CG  PHE D 513     155.565  15.091  30.632  1.00 52.04      D
ATOM   7593  CD1 PHE D 513     154.849  14.187  29.856  1.00 52.52      D
ATOM   7594  CD2 PHE D 513     155.724  16.392  30.164  1.00 51.87      D
ATOM   7595  CE1 PHE D 513     154.305  14.571  28.635  1.00 52.41      D
ATOM   7596  CE2 PHE D 513     155.182  16.785  28.944  1.00 51.44      D
ATOM   7597  CZ  PHE D 513     154.472  15.873  28.181  1.00 51.72      D
ATOM   7598  C   PHE D 513     157.807  13.318  33.225  1.00 52.58      D
ATOM   7599  O   PHE D 513     156.957  13.164  34.100  1.00 53.73      D
ATOM   7600  N   HIS D 514     159.107  13.108  33.427  1.00 52.88      D
ATOM   7601  CA  HIS D 514     159.649  12.656  34.707  1.00 52.63      D
ATOM   7602  CB  HIS D 514     161.150  12.425  34.577  1.00 52.45      D
ATOM   7603  CG  HIS D 514     161.495  11.297  33.662  1.00 53.43      D
ATOM   7604  CD2 HIS D 514     161.857  11.285  32.358  1.00 53.76      D
ATOM   7605  ND1 HIS D 514     161.411   9.977  34.049  1.00 54.13      D
ATOM   7606  CE1 HIS D 514     161.705   9.199  33.023  1.00 54.22      D
ATOM   7607  NE2 HIS D 514     161.979   9.968  31.985  1.00 55.05      D
ATOM   7608  C   HIS D 514     159.388  13.615  35.855  1.00 53.18      D
ATOM   7609  O   HIS D 514     159.096  13.204  36.986  1.00 54.06      D
ATOM   7610  N   THR D 515     159.494  14.901  35.569  1.00 52.64      D
ATOM   7611  CA  THR D 515     159.281  15.888  36.597  1.00 52.40      D
```

```
ATOM   7612  CB  THR D 515     160.524  16.788  36.742  1.00 52.48      D
ATOM   7613  OG1 THR D 515     160.166  17.996  37.420  1.00 52.59      D
ATOM   7614  CG2 THR D 515     161.126  17.093  35.381  1.00 52.87      D
ATOM   7615  C   THR D 515     158.029  16.705  36.322  1.00 52.17      D
ATOM   7616  O   THR D 515     157.858  17.269  35.245  1.00 51.18      D
ATOM   7617  N   PRO D 516     157.114  16.736  37.304  1.00 53.39      D
ATOM   7618  CD  PRO D 516     157.164  15.841  38.478  1.00 53.89      D
ATOM   7619  CA  PRO D 516     155.835  17.449  37.271  1.00 52.84      D
ATOM   7620  CB  PRO D 516     155.231  17.119  38.632  1.00 52.59      D
ATOM   7621  CG  PRO D 516     155.703  15.729  38.851  1.00 52.83      D
ATOM   7622  C   PRO D 516     155.976  18.939  37.057  1.00 51.67      D
ATOM   7623  O   PRO D 516     155.238  19.533  36.279  1.00 52.06      D
ATOM   7624  N   GLU D 517     156.925  19.545  37.751  1.00 51.53      D
ATOM   7625  CA  GLU D 517     157.115  20.974  37.615  1.00 51.30      D
ATOM   7626  CB  GLU D 517     158.171  21.456  38.611  1.00 53.01      D
ATOM   7627  CG  GLU D 517     157.783  21.225  40.076  1.00 55.65      D
ATOM   7628  CD  GLU D 517     156.339  21.648  40.384  1.00 57.61      D
ATOM   7629  OE1 GLU D 517     155.899  22.718  39.901  1.00 58.27      D
ATOM   7630  OE2 GLU D 517     155.641  20.911  41.115  1.00 58.41      D
ATOM   7631  C   GLU D 517     157.482  21.376  36.180  1.00 50.73      D
ATOM   7632  O   GLU D 517     157.417  22.549  35.824  1.00 50.38      D
ATOM   7633  N   GLU D 518     157.853  20.408  35.350  1.00 49.94      D
ATOM   7634  CA  GLU D 518     158.200  20.707  33.964  1.00 48.95      D
ATOM   7635  CB  GLU D 518     159.552  20.081  33.613  1.00 49.87      D
ATOM   7636  CG  GLU D 518     160.741  20.801  34.239  1.00 51.31      D
ATOM   7637  CD  GLU D 518     162.074  20.125  33.945  1.00 52.52      D
ATOM   7638  OE1 GLU D 518     162.225  19.579  32.823  1.00 53.98      D
ATOM   7639  OE2 GLU D 518     162.971  20.153  34.826  1.00 50.01      D
ATOM   7640  C   GLU D 518     157.119  20.209  33.003  1.00 47.92      D
ATOM   7641  O   GLU D 518     157.143  20.496  31.808  1.00 47.01      D
ATOM   7642  N   ASN D 519     156.164  19.465  33.541  1.00 47.59      D
ATOM   7643  CA  ASN D 519     155.071  18.933  32.746  1.00 46.99      D
ATOM   7644  CB  ASN D 519     154.490  17.710  33.459  1.00 45.93      D
ATOM   7645  CG  ASN D 519     153.454  16.995  32.633  1.00 45.28      D
ATOM   7646  OD1 ASN D 519     152.907  15.970  33.055  1.00 45.38      D
ATOM   7647  ND2 ASN D 519     153.173  17.526  31.445  1.00 42.56      D
ATOM   7648  C   ASN D 519     153.998  20.023  32.551  1.00 46.69      D
ATOM   7649  O   ASN D 519     153.408  20.516  33.524  1.00 46.92      D
ATOM   7650  N   PRO D 520     153.758  20.431  31.291  1.00 45.28      D
ATOM   7651  CD  PRO D 520     154.544  20.037  30.110  1.00 43.44      D
ATOM   7652  CA  PRO D 520     152.769  21.460  30.937  1.00 44.93      D
ATOM   7653  CB  PRO D 520     152.965  21.621  29.431  1.00 43.10      D
ATOM   7654  CG  PRO D 520     154.396  21.232  29.234  1.00 43.83      D
ATOM   7655  C   PRO D 520     151.328  21.058  31.265  1.00 44.42      D
ATOM   7656  O   PRO D 520     150.430  21.899  31.341  1.00 45.05      D
ATOM   7657  N   TYR D 521     151.126  19.764  31.465  1.00 43.22      D
ATOM   7658  CA  TYR D 521     149.808  19.216  31.733  1.00 42.86      D
ATOM   7659  CB  TYR D 521     149.707  17.885  31.017  1.00 42.46      D
ATOM   7660  CG  TYR D 521     150.006  17.994  29.543  1.00 41.84      D
ATOM   7661  CD1 TYR D 521     149.117  18.639  28.684  1.00 43.00      D
ATOM   7662  CE1 TYR D 521     149.330  18.673  27.315  1.00 42.26      D
ATOM   7663  CD2 TYR D 521     151.135  17.395  28.996  1.00 42.03      D
ATOM   7664  CE2 TYR D 521     151.363  17.422  27.625  1.00 42.28      D
ATOM   7665  CZ  TYR D 521     150.445  18.058  26.788  1.00 43.30      D
```

```
ATOM   7666  OH  TYR D 521     150.592  18.015  25.418  1.00 44.00      D
ATOM   7667  C   TYR D 521     149.444  19.047  33.211  1.00 42.72      D
ATOM   7668  O   TYR D 521     148.267  18.922  33.567  1.00 42.06      D
ATOM   7669  N   PHE D 522     150.459  19.030  34.065  1.00 41.61      D
ATOM   7670  CA  PHE D 522     150.263  18.902  35.500  1.00 40.23      D
ATOM   7671  CB  PHE D 522     151.606  18.630  36.163  1.00 40.93      D
ATOM   7672  CG  PHE D 522     151.580  18.761  37.646  1.00 41.77      D
ATOM   7673  CD1 PHE D 522     150.784  17.923  38.415  1.00 42.70      D
ATOM   7674  CD2 PHE D 522     152.362  19.716  38.280  1.00 42.48      D
ATOM   7675  CE1 PHE D 522     150.770  18.030  39.800  1.00 43.11      D
ATOM   7676  CE2 PHE D 522     152.357  19.835  39.665  1.00 43.56      D
ATOM   7677  CZ  PHE D 522     151.559  18.989  40.427  1.00 44.10      D
ATOM   7678  C   PHE D 522     149.682  20.218  36.013  1.00 38.95      D
ATOM   7679  O   PHE D 522     149.994  21.271  35.470  1.00 38.64      D
ATOM   7680  N   VAL D 523     148.823  20.169  37.028  1.00 38.34      D
ATOM   7681  CA  VAL D 523     148.256  21.407  37.559  1.00 38.44      D
ATOM   7682  CB  VAL D 523     146.720  21.500  37.351  1.00 37.33      D
ATOM   7683  CG1 VAL D 523     146.352  21.189  35.900  1.00 35.81      D
ATOM   7684  CG2 VAL D 523     146.020  20.585  38.298  1.00 39.53      D
ATOM   7685  C   VAL D 523     148.543  21.590  39.044  1.00 38.09      D
ATOM   7686  O   VAL D 523     148.774  22.712  39.510  1.00 38.38      D
ATOM   7687  N   GLY D 524     148.543  20.484  39.780  1.00 36.48      D
ATOM   7688  CA  GLY D 524     148.798  20.567  41.203  1.00 35.67      D
ATOM   7689  C   GLY D 524     148.389  19.349  42.012  1.00 34.74      D
ATOM   7690  O   GLY D 524     147.705  18.446  41.512  1.00 36.14      D
ATOM   7691  N   VAL D 525     148.812  19.351  43.276  1.00 32.26      D
ATOM   7692  CA  VAL D 525     148.563  18.270  44.224  1.00 28.84      D
ATOM   7693  CB  VAL D 525     149.834  17.940  44.980  1.00 28.68      D
ATOM   7694  CG1 VAL D 525     149.536  16.914  46.060  1.00 28.23      D
ATOM   7695  CG2 VAL D 525     150.913  17.467  43.993  1.00 27.71      D
ATOM   7696  C   VAL D 525     147.522  18.613  45.261  1.00 27.86      D
ATOM   7697  O   VAL D 525     147.686  19.580  45.985  1.00 29.26      D
ATOM   7698  N   LEU D 526     146.469  17.807  45.349  1.00 26.79      D
ATOM   7699  CA  LEU D 526     145.421  18.028  46.341  1.00 24.97      D
ATOM   7700  CB  LEU D 526     144.082  17.539  45.796  1.00 24.09      D
ATOM   7701  CG  LEU D 526     143.105  18.496  45.072  1.00 25.53      D
ATOM   7702  CD1 LEU D 526     143.706  19.861  44.714  1.00 21.96      D
ATOM   7703  CD2 LEU D 526     142.600  17.770  43.842  1.00 24.82      D
ATOM   7704  C   LEU D 526     145.771  17.305  47.659  1.00 25.98      D
ATOM   7705  O   LEU D 526     145.389  16.153  47.865  1.00 26.01      D
ATOM   7706  N   ARG D 527     146.507  18.008  48.533  1.00 26.45      D
ATOM   7707  CA  ARG D 527     146.953  17.504  49.839  1.00 27.15      D
ATOM   7708  CB  ARG D 527     148.068  18.359  50.423  1.00 29.53      D
ATOM   7709  CG  ARG D 527     149.136  18.793  49.481  1.00 30.78      D
ATOM   7710  CD  ARG D 527     150.199  17.750  49.353  1.00 29.79      D
ATOM   7711  NE  ARG D 527     151.289  18.254  48.534  1.00 28.82      D
ATOM   7712  CZ  ARG D 527     152.426  17.609  48.341  1.00 28.06      D
ATOM   7713  NH1 ARG D 527     152.621  16.424  48.913  1.00 27.74      D
ATOM   7714  NH2 ARG D 527     153.361  18.156  47.578  1.00 28.96      D
ATOM   7715  C   ARG D 527     145.833  17.583  50.854  1.00 27.48      D
ATOM   7716  O   ARG D 527     145.198  18.625  50.982  1.00 28.10      D
ATOM   7717  N   GLY D 528     145.643  16.511  51.618  1.00 27.13      D
ATOM   7718  CA  GLY D 528     144.593  16.502  52.618  1.00 25.97      D
ATOM   7719  C   GLY D 528     144.378  15.186  53.350  1.00 27.12      D
```

```
ATOM   7720  O   GLY D 528     144.222  15.170  54.573  1.00 26.85      D
ATOM   7721  N   HIS D 529     144.349  14.076  52.619  1.00 28.35      D
ATOM   7722  CA  HIS D 529     144.148  12.771  53.242  1.00 28.78      D
ATOM   7723  CB  HIS D 529     143.686  11.747  52.197  1.00 29.36      D
ATOM   7724  CG  HIS D 529     142.272  11.942  51.729  1.00 31.01      D
ATOM   7725  CD2 HIS D 529     141.776  12.234  50.502  1.00 32.50      D
ATOM   7726  ND1 HIS D 529     141.181  11.808  52.562  1.00 29.94      D
ATOM   7727  CE1 HIS D 529     140.074  12.010  51.864  1.00 32.77      D
ATOM   7728  NE2 HIS D 529     140.409  12.270  50.613  1.00 31.73      D
ATOM   7729  C   HIS D 529     145.428  12.293  53.922  1.00 29.06      D
ATOM   7730  O   HIS D 529     146.525  12.716  53.562  1.00 29.97      D
ATOM   7731  N   MSE D 530     145.278  11.412  54.906  1.00 30.41      D
ATOM   7732  CA  MSE D 530     146.411  10.872  55.662  1.00 31.44      D
ATOM   7733  CB  MSE D 530     146.116  10.979  57.163  1.00 36.54      D
ATOM   7734  CG  MSE D 530     145.727  12.383  57.647  1.00 40.77      D
ATOM   7735  SE  MSE D 530     147.225  13.555  57.992  1.00 48.72      D
ATOM   7736  CE  MSE D 530     147.747  12.886  59.726  1.00 44.45      D
ATOM   7737  C   MSE D 530     146.708   9.409  55.286  1.00 30.15      D
ATOM   7738  O   MSE D 530     147.663   8.804  55.770  1.00 31.06      D
ATOM   7739  N   ALA D 531     145.872   8.837  54.433  1.00 27.91      D
ATOM   7740  CA  ALA D 531     146.077   7.470  53.983  1.00 25.52      D
ATOM   7741  CB  ALA D 531     145.322   6.506  54.863  1.00 23.17      D
ATOM   7742  C   ALA D 531     145.634   7.329  52.528  1.00 25.05      D
ATOM   7743  O   ALA D 531     145.166   8.283  51.903  1.00 25.19      D
ATOM   7744  N   SER D 532     145.778   6.126  52.004  1.00 24.01      D
ATOM   7745  CA  SER D 532     145.431   5.834  50.635  1.00 23.62      D
ATOM   7746  CB  SER D 532     145.452   4.332  50.427  1.00 23.66      D
ATOM   7747  OG  SER D 532     145.044   4.009  49.120  1.00 24.72      D
ATOM   7748  C   SER D 532     144.093   6.391  50.161  1.00 24.24      D
ATOM   7749  O   SER D 532     143.059   6.249  50.835  1.00 23.67      D
ATOM   7750  N   VAL D 533     144.131   7.028  48.987  1.00 22.26      D
ATOM   7751  CA  VAL D 533     142.930   7.588  48.383  1.00 21.80      D
ATOM   7752  CB  VAL D 533     143.238   8.790  47.509  1.00 19.37      D
ATOM   7753  CG1 VAL D 533     141.973   9.225  46.786  1.00 19.14      D
ATOM   7754  CG2 VAL D 533     143.757   9.912  48.367  1.00 16.33      D
ATOM   7755  C   VAL D 533     142.311   6.476  47.564  1.00 23.09      D
ATOM   7756  O   VAL D 533     142.740   6.181  46.464  1.00 24.67      D
ATOM   7757  N   ARG D 534     141.281   5.865  48.125  1.00 23.37      D
ATOM   7758  CA  ARG D 534     140.630   4.734  47.514  1.00 21.94      D
ATOM   7759  CB  ARG D 534     139.887   3.966  48.588  1.00 22.94      D
ATOM   7760  CG  ARG D 534     139.334   2.660  48.104  1.00 20.89      D
ATOM   7761  CD  ARG D 534     140.460   1.735  47.688  1.00 20.13      D
ATOM   7762  NE  ARG D 534     139.934   0.404  47.470  1.00 22.05      D
ATOM   7763  CZ  ARG D 534     139.177   0.061  46.435  1.00 21.88      D
ATOM   7764  NH1 ARG D 534     138.859   0.955  45.499  1.00 16.38      D
ATOM   7765  NH2 ARG D 534     138.723  -1.184  46.354  1.00 21.24      D
ATOM   7766  C   ARG D 534     139.687   4.934  46.350  1.00 21.77      D
ATOM   7767  O   ARG D 534     139.630   4.082  45.464  1.00 23.87      D
ATOM   7768  N   THR D 535     138.944   6.029  46.328  1.00 21.46      D
ATOM   7769  CA  THR D 535     137.976   6.186  45.252  1.00 23.21      D
ATOM   7770  CB  THR D 535     136.630   5.607  45.693  1.00 22.72      D
ATOM   7771  OG1 THR D 535     135.615   5.908  44.728  1.00 24.25      D
ATOM   7772  CG2 THR D 535     136.255   6.189  47.038  1.00 21.59      D
ATOM   7773  C   THR D 535     137.785   7.623  44.871  1.00 22.36      D
```

```
ATOM   7774  O   THR D 535     138.010   8.494  45.692  1.00 22.27      D
ATOM   7775  N   VAL D 536     137.383   7.869  43.627  1.00 23.47      D
ATOM   7776  CA  VAL D 536     137.154   9.240  43.178  1.00 26.56      D
ATOM   7777  CB  VAL D 536     138.340   9.805  42.381  1.00 27.30      D
ATOM   7778  CG1 VAL D 536     138.152  11.303  42.178  1.00 27.76      D
ATOM   7779  CG2 VAL D 536     139.615   9.573  43.126  1.00 29.04      D
ATOM   7780  C   VAL D 536     135.907   9.379  42.330  1.00 26.74      D
ATOM   7781  O   VAL D 536     135.550   8.486  41.558  1.00 28.31      D
ATOM   7782  N   SER D 537     135.248  10.517  42.473  1.00 26.29      D
ATOM   7783  CA  SER D 537     134.019  10.759  41.741  1.00 25.58      D
ATOM   7784  CB  SER D 537     132.832  10.197  42.529  1.00 23.69      D
ATOM   7785  OG  SER D 537     131.605  10.436  41.878  1.00 19.22      D
ATOM   7786  C   SER D 537     133.859  12.252  41.547  1.00 26.69      D
ATOM   7787  O   SER D 537     133.697  13.000  42.517  1.00 27.22      D
ATOM   7788  N   GLY D 538     133.923  12.684  40.294  1.00 26.82      D
ATOM   7789  CA  GLY D 538     133.794  14.096  40.020  1.00 28.64      D
ATOM   7790  C   GLY D 538     133.027  14.446  38.766  1.00 28.83      D
ATOM   7791  O   GLY D 538     132.961  13.666  37.820  1.00 29.17      D
ATOM   7792  N   HIS D 539     132.450  15.645  38.790  1.00 29.15      D
ATOM   7793  CA  HIS D 539     131.679  16.226  37.696  1.00 27.88      D
ATOM   7794  CB  HIS D 539     130.179  16.025  37.911  1.00 27.43      D
ATOM   7795  CG  HIS D 539     129.333  16.567  36.799  1.00 28.11      D
ATOM   7796  CD2 HIS D 539     128.736  17.772  36.637  1.00 30.46      D
ATOM   7797  ND1 HIS D 539     129.046  15.843  35.662  1.00 27.67      D
ATOM   7798  CE1 HIS D 539     128.307  16.577  34.848  1.00 29.05      D
ATOM   7799  NE2 HIS D 539     128.105  17.753  35.415  1.00 30.92      D
ATOM   7800  C   HIS D 539     131.959  17.735  37.697  1.00 29.12      D
ATOM   7801  O   HIS D 539     131.791  18.409  38.728  1.00 28.57      D
ATOM   7802  N   GLY D 540     132.376  18.261  36.546  1.00 28.54      D
ATOM   7803  CA  GLY D 540     132.650  19.682  36.436  1.00 27.08      D
ATOM   7804  C   GLY D 540     133.872  20.122  37.215  1.00 27.09      D
ATOM   7805  O   GLY D 540     134.904  19.454  37.179  1.00 28.54      D
ATOM   7806  N   ASN D 541     133.777  21.245  37.920  1.00 25.16      D
ATOM   7807  CA  ASN D 541     134.924  21.706  38.679  1.00 24.86      D
ATOM   7808  CB  ASN D 541     134.907  23.237  38.816  1.00 26.35      D
ATOM   7809  CG  ASN D 541     133.889  23.726  39.851  1.00 29.47      D
ATOM   7810  OD1 ASN D 541     132.706  23.341  39.803  1.00 29.21      D
ATOM   7811  ND2 ASN D 541     134.341  24.575  40.792  1.00 26.35      D
ATOM   7812  C   ASN D 541     134.915  21.062  40.056  1.00 24.63      D
ATOM   7813  O   ASN D 541     135.803  21.308  40.864  1.00 25.54      D
ATOM   7814  N   ILE D 542     133.921  20.220  40.321  1.00 22.93      D
ATOM   7815  CA  ILE D 542     133.821  19.574  41.629  1.00 22.46      D
ATOM   7816  CB  ILE D 542     132.361  19.724  42.186  1.00 20.91      D
ATOM   7817  CG2 ILE D 542     132.215  18.977  43.497  1.00 22.05      D
ATOM   7818  CG1 ILE D 542     132.001  21.215  42.385  1.00 19.70      D
ATOM   7819  CD1 ILE D 542     132.866  22.016  43.388  1.00 10.85      D
ATOM   7820  C   ILE D 542     134.258  18.085  41.663  1.00 24.27      D
ATOM   7821  O   ILE D 542     133.841  17.258  40.832  1.00 23.68      D
ATOM   7822  N   VAL D 543     135.108  17.738  42.624  1.00 24.95      D
ATOM   7823  CA  VAL D 543     135.565  16.350  42.735  1.00 26.33      D
ATOM   7824  CB  VAL D 543     137.023  16.176  42.199  1.00 28.00      D
ATOM   7825  CG1 VAL D 543     137.492  14.742  42.406  1.00 27.16      D
ATOM   7826  CG2 VAL D 543     137.073  16.515  40.716  1.00 30.18      D
ATOM   7827  C   VAL D 543     135.509  15.864  44.174  1.00 25.02      D
```

```
ATOM   7828  O   VAL D 543     135.893  16.601  45.079  1.00 24.45      D
ATOM   7829  N   VAL D 544     135.017  14.639  44.388  1.00 24.93      D
ATOM   7830  CA  VAL D 544     134.939  14.093  45.748  1.00 25.31      D
ATOM   7831  CB  VAL D 544     133.495  13.783  46.197  1.00 24.60      D
ATOM   7832  CG1 VAL D 544     133.507  13.509  47.679  1.00 24.71      D
ATOM   7833  CG2 VAL D 544     132.553  14.940  45.889  1.00 25.25      D
ATOM   7834  C   VAL D 544     135.750  12.814  45.910  1.00 25.25      D
ATOM   7835  O   VAL D 544     135.662  11.903  45.082  1.00 26.67      D
ATOM   7836  N   SER D 545     136.534  12.745  46.985  1.00 24.15      D
ATOM   7837  CA  SER D 545     137.367  11.566  47.236  1.00 24.66      D
ATOM   7838  CB  SER D 545     138.835  11.960  47.213  1.00 22.85      D
ATOM   7839  OG  SER D 545     139.110  12.914  48.221  1.00 26.17      D
ATOM   7840  C   SER D 545     137.105  10.777  48.525  1.00 26.03      D
ATOM   7841  O   SER D 545     136.609  11.315  49.516  1.00 27.76      D
ATOM   7842  N   GLY D 546     137.467   9.497  48.495  1.00 25.26      D
ATOM   7843  CA  GLY D 546     137.292   8.642  49.647  1.00 24.44      D
ATOM   7844  C   GLY D 546     138.637   8.073  50.039  1.00 24.54      D
ATOM   7845  O   GLY D 546     139.318   7.450  49.220  1.00 23.24      D
ATOM   7846  N   SER D 547     139.038   8.282  51.288  1.00 25.20      D
ATOM   7847  CA  SER D 547     140.339   7.773  51.730  1.00 27.40      D
ATOM   7848  CB  SER D 547     141.235   8.897  52.239  1.00 25.06      D
ATOM   7849  OG  SER D 547     142.424   8.333  52.763  1.00 23.13      D
ATOM   7850  C   SER D 547     140.286   6.723  52.816  1.00 28.75      D
ATOM   7851  O   SER D 547     139.260   6.520  53.462  1.00 32.39      D
ATOM   7852  N   TYR D 548     141.411   6.062  53.031  1.00 27.35      D
ATOM   7853  CA  TYR D 548     141.457   5.071  54.078  1.00 24.34      D
ATOM   7854  CB  TYR D 548     142.588   4.085  53.835  1.00 21.23      D
ATOM   7855  CG  TYR D 548     142.185   2.933  52.964  1.00 18.24      D
ATOM   7856  CD1 TYR D 548     140.975   2.940  52.267  1.00 17.37      D
ATOM   7857  CE1 TYR D 548     140.631   1.894  51.426  1.00 15.22      D
ATOM   7858  CD2 TYR D 548     143.030   1.850  52.802  1.00 18.07      D
ATOM   7859  CE2 TYR D 548     142.701   0.796  51.969  1.00 15.33      D
ATOM   7860  CZ  TYR D 548     141.507   0.825  51.283  1.00 17.35      D
ATOM   7861  OH  TYR D 548     141.195  -0.213  50.435  1.00 18.41      D
ATOM   7862  C   TYR D 548     141.637   5.742  55.428  1.00 25.52      D
ATOM   7863  O   TYR D 548     141.897   5.060  56.401  1.00 24.80      D
ATOM   7864  N   ASP D 549     141.517   7.070  55.496  1.00 26.28      D
ATOM   7865  CA  ASP D 549     141.637   7.739  56.789  1.00 26.66      D
ATOM   7866  CB  ASP D 549     142.332   9.114  56.693  1.00 28.11      D
ATOM   7867  CG  ASP D 549     141.761  10.006  55.611  1.00 28.18      D
ATOM   7868  OD1 ASP D 549     140.580   9.822  55.227  1.00 30.65      D
ATOM   7869  OD2 ASP D 549     142.507  10.909  55.167  1.00 25.41      D
ATOM   7870  C   ASP D 549     140.239   7.884  57.363  1.00 26.46      D
ATOM   7871  O   ASP D 549     140.014   8.634  58.311  1.00 26.79      D
ATOM   7872  N   ASN D 550     139.309   7.157  56.742  1.00 26.14      D
ATOM   7873  CA  ASN D 550     137.906   7.115  57.139  1.00 24.53      D
ATOM   7874  CB  ASN D 550     137.825   6.849  58.633  1.00 23.45      D
ATOM   7875  CG  ASN D 550     138.484   5.542  59.012  1.00 23.88      D
ATOM   7876  OD1 ASN D 550     139.126   4.894  58.190  1.00 24.66      D
ATOM   7877  ND2 ASN D 550     138.319   5.143  60.253  1.00 25.10      D
ATOM   7878  C   ASN D 550     137.162   8.374  56.796  1.00 23.51      D
ATOM   7879  O   ASN D 550     136.006   8.534  57.146  1.00 23.99      D
ATOM   7880  N   THR D 551     137.811   9.237  56.038  1.00 24.61      D
ATOM   7881  CA  THR D 551     137.221  10.510  55.706  1.00 24.98      D
```

```
ATOM   7882  CB  THR D 551     138.155  11.584  56.208  1.00 25.84      D
ATOM   7883  OG1 THR D 551     137.402  12.640  56.803  1.00 26.76      D
ATOM   7884  CG2 THR D 551     139.015  12.107  55.053  1.00 24.97      D
ATOM   7885  C   THR D 551     136.993  10.725  54.206  1.00 25.92      D
ATOM   7886  O   THR D 551     137.535   9.996  53.376  1.00 24.99      D
ATOM   7887  N   LEU D 552     136.173  11.719  53.868  1.00 26.68      D
ATOM   7888  CA  LEU D 552     135.934  12.079  52.471  1.00 26.79      D
ATOM   7889  CB  LEU D 552     134.508  11.771  52.031  1.00 24.86      D
ATOM   7890  CG  LEU D 552     134.189  10.328  51.665  1.00 23.77      D
ATOM   7891  CD1 LEU D 552     133.215   9.804  52.689  1.00 23.78      D
ATOM   7892  CD2 LEU D 552     133.597  10.237  50.257  1.00 22.54      D
ATOM   7893  C   LEU D 552     136.180  13.572  52.308  1.00 27.51      D
ATOM   7894  O   LEU D 552     135.792  14.366  53.170  1.00 28.40      D
ATOM   7895  N   ILE D 553     136.828  13.955  51.206  1.00 27.13      D
ATOM   7896  CA  ILE D 553     137.102  15.372  50.939  1.00 25.65      D
ATOM   7897  CB  ILE D 553     138.623  15.686  50.957  1.00 24.82      D
ATOM   7898  CG2 ILE D 553     138.854  17.153  50.606  1.00 24.33      D
ATOM   7899  CG1 ILE D 553     139.212  15.444  52.355  1.00 25.26      D
ATOM   7900  CD1 ILE D 553     140.725  15.613  52.413  1.00 24.18      D
ATOM   7901  C   ILE D 553     136.531  15.869  49.606  1.00 25.82      D
ATOM   7902  O   ILE D 553     136.664  15.210  48.561  1.00 24.35      D
ATOM   7903  N   VAL D 554     135.889  17.038  49.672  1.00 24.96      D
ATOM   7904  CA  VAL D 554     135.299  17.704  48.503  1.00 24.79      D
ATOM   7905  CB  VAL D 554     133.964  18.425  48.858  1.00 21.69      D
ATOM   7906  CG1 VAL D 554     133.366  19.041  47.620  1.00 19.43      D
ATOM   7907  CG2 VAL D 554     133.000  17.455  49.480  1.00 21.35      D
ATOM   7908  C   VAL D 554     136.308  18.753  48.016  1.00 26.46      D
ATOM   7909  O   VAL D 554     136.646  19.689  48.746  1.00 26.64      D
ATOM   7910  N   TRP D 555     136.812  18.574  46.797  1.00 27.69      D
ATOM   7911  CA  TRP D 555     137.784  19.500  46.233  1.00 28.09      D
ATOM   7912  CB  TRP D 555     139.026  18.767  45.703  1.00 28.18      D
ATOM   7913  CG  TRP D 555     139.593  17.681  46.576  1.00 29.63      D
ATOM   7914  CD2 TRP D 555     140.695  17.795  47.487  1.00 30.60      D
ATOM   7915  CE2 TRP D 555     140.948  16.505  48.003  1.00 30.79      D
ATOM   7916  CE3 TRP D 555     141.492  18.862  47.915  1.00 30.24      D
ATOM   7917  CD1 TRP D 555     139.228  16.365  46.587  1.00 29.55      D
ATOM   7918  NE1 TRP D 555     140.041  15.652  47.436  1.00 30.90      D
ATOM   7919  CZ2 TRP D 555     141.968  16.253  48.921  1.00 31.50      D
ATOM   7920  CZ3 TRP D 555     142.510  18.608  48.832  1.00 31.00      D
ATOM   7921  CH2 TRP D 555     142.736  17.314  49.323  1.00 31.35      D
ATOM   7922  C   TRP D 555     137.210  20.306  45.075  1.00 27.75      D
ATOM   7923  O   TRP D 555     136.392  19.807  44.297  1.00 26.08      D
ATOM   7924  N   ASP D 556     137.658  21.556  44.981  1.00 29.07      D
ATOM   7925  CA  ASP D 556     137.274  22.463  43.904  1.00 29.82      D
ATOM   7926  CB  ASP D 556     136.917  23.849  44.425  1.00 33.43      D
ATOM   7927  CG  ASP D 556     136.336  24.762  43.335  1.00 36.51      D
ATOM   7928  OD1 ASP D 556     136.913  24.864  42.216  1.00 35.80      D
ATOM   7929  OD2 ASP D 556     135.285  25.388  43.609  1.00 39.49      D
ATOM   7930  C   ASP D 556     138.539  22.591  43.095  1.00 28.83      D
ATOM   7931  O   ASP D 556     139.440  23.337  43.463  1.00 25.39      D
ATOM   7932  N   VAL D 557     138.596  21.858  41.995  1.00 31.59      D
ATOM   7933  CA  VAL D 557     139.756  21.853  41.123  1.00 34.16      D
ATOM   7934  CB  VAL D 557     139.592  20.840  40.007  1.00 34.22      D
ATOM   7935  CG1 VAL D 557     140.777  20.942  39.064  1.00 36.74      D
```

```
ATOM   7936  CG2 VAL D 557     139.460  19.444  40.582  1.00 31.24      D
ATOM   7937  C   VAL D 557     140.021  23.183  40.466  1.00 35.74      D
ATOM   7938  O   VAL D 557     141.168  23.535  40.244  1.00 37.94      D
ATOM   7939  N   ALA D 558     138.959  23.906  40.133  1.00 37.02      D
ATOM   7940  CA  ALA D 558     139.107  25.196  39.485  1.00 37.13      D
ATOM   7941  CB  ALA D 558     137.747  25.730  39.065  1.00 39.25      D
ATOM   7942  C   ALA D 558     139.784  26.167  40.430  1.00 36.58      D
ATOM   7943  O   ALA D 558     140.342  27.168  39.997  1.00 37.02      D
ATOM   7944  N   GLN D 559     139.729  25.857  41.722  1.00 37.85      D
ATOM   7945  CA  GLN D 559     140.327  26.688  42.763  1.00 37.56      D
ATOM   7946  CB  GLN D 559     139.248  27.110  43.750  1.00 37.90      D
ATOM   7947  CG  GLN D 559     139.672  28.264  44.624  1.00 43.44      D
ATOM   7948  CD  GLN D 559     138.523  28.874  45.444  1.00 45.28      D
ATOM   7949  OE1 GLN D 559     137.375  28.927  44.987  1.00 46.49      D
ATOM   7950  NE2 GLN D 559     138.839  29.354  46.655  1.00 45.82      D
ATOM   7951  C   GLN D 559     141.419  25.896  43.479  1.00 37.70      D
ATOM   7952  O   GLN D 559     142.131  26.428  44.336  1.00 36.85      D
ATOM   7953  N   MSE D 560     141.535  24.624  43.094  1.00 38.22      D
ATOM   7954  CA  MSE D 560     142.505  23.687  43.645  1.00 37.94      D
ATOM   7955  CB  MSE D 560     143.870  23.912  42.984  1.00 37.36      D
ATOM   7956  CG  MSE D 560     144.681  22.648  42.719  1.00 37.70      D
ATOM   7957  SE  MSE D 560     143.786  21.540  41.377  1.00 39.17      D
ATOM   7958  CE  MSE D 560     143.835  22.738  39.886  1.00 41.26      D
ATOM   7959  C   MSE D 560     142.597  23.865  45.164  1.00 37.81      D
ATOM   7960  O   MSE D 560     143.675  24.035  45.710  1.00 39.53      D
ATOM   7961  N   LYS D 561     141.449  23.844  45.832  1.00 37.74      D
ATOM   7962  CA  LYS D 561     141.384  23.995  47.279  1.00 38.73      D
ATOM   7963  CB  LYS D 561     141.037  25.452  47.638  1.00 39.81      D
ATOM   7964  CG  LYS D 561     142.191  26.428  47.399  0.00 40.07      D
ATOM   7965  CD  LYS D 561     143.372  26.124  48.318  0.00 40.65      D
ATOM   7966  CE  LYS D 561     142.998  26.355  49.774  0.00 41.01      D
ATOM   7967  NZ  LYS D 561     144.024  25.827  50.715  0.00 41.29      D
ATOM   7968  C   LYS D 561     140.356  23.022  47.887  1.00 39.22      D
ATOM   7969  O   LYS D 561     139.419  22.584  47.208  1.00 38.84      D
ATOM   7970  N   CYS D 562     140.556  22.670  49.159  1.00 38.90      D
ATOM   7971  CA  CYS D 562     139.668  21.759  49.885  1.00 38.52      D
ATOM   7972  CB  CYS D 562     140.360  21.270  51.164  1.00 38.67      D
ATOM   7973  SG  CYS D 562     139.309  20.275  52.277  1.00 44.51      D
ATOM   7974  C   CYS D 562     138.402  22.521  50.260  1.00 37.58      D
ATOM   7975  O   CYS D 562     138.494  23.572  50.888  1.00 40.09      D
ATOM   7976  N   LEU D 563     137.223  22.015  49.895  1.00 34.69      D
ATOM   7977  CA  LEU D 563     135.981  22.726  50.232  1.00 31.60      D
ATOM   7978  CB  LEU D 563     134.924  22.550  49.132  1.00 28.39      D
ATOM   7979  CG  LEU D 563     135.214  23.279  47.820  1.00 25.92      D
ATOM   7980  CD1 LEU D 563     133.986  23.317  46.939  1.00 24.65      D
ATOM   7981  CD2 LEU D 563     135.679  24.670  48.139  1.00 23.99      D
ATOM   7982  C   LEU D 563     135.388  22.281  51.552  1.00 30.82      D
ATOM   7983  O   LEU D 563     135.012  23.099  52.388  1.00 29.72      D
ATOM   7984  N   TYR D 564     135.320  20.968  51.723  1.00 31.20      D
ATOM   7985  CA  TYR D 564     134.768  20.358  52.915  1.00 29.79      D
ATOM   7986  CB  TYR D 564     133.276  20.087  52.705  1.00 31.53      D
ATOM   7987  CG  TYR D 564     132.415  21.316  52.480  1.00 35.18      D
ATOM   7988  CD1 TYR D 564     132.216  22.250  53.503  1.00 35.47      D
ATOM   7989  CE1 TYR D 564     131.381  23.356  53.321  1.00 37.11      D
```

```
ATOM   7990  CD2 TYR D 564     131.757  21.522  51.257  1.00 35.79      D
ATOM   7991  CE2 TYR D 564     130.918  22.626  51.064  1.00 37.32      D
ATOM   7992  CZ  TYR D 564     130.733  23.539  52.100  1.00 37.56      D
ATOM   7993  OH  TYR D 564     129.901  24.625  51.926  1.00 37.99      D
ATOM   7994  C   TYR D 564     135.464  19.028  53.213  1.00 28.42      D
ATOM   7995  O   TYR D 564     135.998  18.357  52.323  1.00 29.93      D
ATOM   7996  N   ILE D 565     135.448  18.655  54.482  1.00 26.22      D
ATOM   7997  CA  ILE D 565     136.001  17.389  54.916  1.00 24.23      D
ATOM   7998  CB  ILE D 565     137.222  17.574  55.861  1.00 24.90      D
ATOM   7999  CG2 ILE D 565     137.641  16.232  56.471  1.00 22.64      D
ATOM   8000  CG1 ILE D 565     138.389  18.173  55.066  1.00 23.83      D
ATOM   8001  CD1 ILE D 565     139.596  18.476  55.898  1.00 22.10      D
ATOM   8002  C   ILE D 565     134.853  16.708  55.654  1.00 24.14      D
ATOM   8003  O   ILE D 565     134.436  17.123  56.745  1.00 24.92      D
ATOM   8004  N   LEU D 566     134.319  15.674  55.022  1.00 23.68      D
ATOM   8005  CA  LEU D 566     133.209  14.910  55.567  1.00 21.44      D
ATOM   8006  CB  LEU D 566     132.498  14.204  54.433  1.00 18.60      D
ATOM   8007  CG  LEU D 566     132.249  15.108  53.240  1.00 16.04      D
ATOM   8008  CD1 LEU D 566     131.493  14.312  52.195  1.00 18.64      D
ATOM   8009  CD2 LEU D 566     131.471  16.327  53.661  1.00 11.95      D
ATOM   8010  C   LEU D 566     133.725  13.876  56.532  1.00 20.93      D
ATOM   8011  O   LEU D 566     134.448  12.975  56.126  1.00 21.77      D
ATOM   8012  N   SER D 567     133.345  13.980  57.800  1.00 22.31      D
ATOM   8013  CA  SER D 567     133.806  12.995  58.783  1.00 23.94      D
ATOM   8014  CB  SER D 567     134.810  13.630  59.731  1.00 23.34      D
ATOM   8015  OG  SER D 567     135.808  14.311  58.987  1.00 24.18      D
ATOM   8016  C   SER D 567     132.676  12.349  59.568  1.00 24.28      D
ATOM   8017  O   SER D 567     131.586  12.904  59.663  1.00 24.81      D
ATOM   8018  N   GLY D 568     132.950  11.166  60.113  1.00 25.74      D
ATOM   8019  CA  GLY D 568     131.953  10.416  60.858  1.00 25.21      D
ATOM   8020  C   GLY D 568     132.134   8.906  60.681  1.00 26.37      D
ATOM   8021  O   GLY D 568     132.130   8.163  61.664  1.00 27.73      D
ATOM   8022  N   HIS D 569     132.288   8.440  59.437  1.00 25.07      D
ATOM   8023  CA  HIS D 569     132.500   7.007  59.175  1.00 23.33      D
ATOM   8024  CB  HIS D 569     132.949   6.749  57.730  1.00 22.22      D
ATOM   8025  CG  HIS D 569     131.839   6.801  56.725  1.00 21.96      D
ATOM   8026  CD2 HIS D 569     131.594   7.675  55.720  1.00 21.82      D
ATOM   8027  ND1 HIS D 569     130.827   5.865  56.671  1.00 20.28      D
ATOM   8028  CE1 HIS D 569     130.009   6.160  55.676  1.00 20.59      D
ATOM   8029  NE2 HIS D 569     130.452   7.254  55.083  1.00 20.12      D
ATOM   8030  C   HIS D 569     133.590   6.520  60.129  1.00 24.25      D
ATOM   8031  O   HIS D 569     134.625   7.176  60.291  1.00 24.38      D
ATOM   8032  N   THR D 570     133.357   5.371  60.759  1.00 25.24      D
ATOM   8033  CA  THR D 570     134.296   4.806  61.724  1.00 25.54      D
ATOM   8034  CB  THR D 570     133.508   4.097  62.867  1.00 26.19      D
ATOM   8035  OG1 THR D 570     132.385   3.381  62.321  1.00 27.58      D
ATOM   8036  CG2 THR D 570     133.008   5.120  63.869  1.00 23.79      D
ATOM   8037  C   THR D 570     135.355   3.864  61.114  1.00 25.50      D
ATOM   8038  O   THR D 570     136.225   3.349  61.812  1.00 26.67      D
ATOM   8039  N   ASP D 571     135.279   3.628  59.811  1.00 26.22      D
ATOM   8040  CA  ASP D 571     136.284   2.804  59.141  1.00 25.18      D
ATOM   8041  CB  ASP D 571     135.810   1.365  58.999  1.00 26.72      D
ATOM   8042  CG  ASP D 571     136.956   0.386  59.009  1.00 28.41      D
ATOM   8043  OD1 ASP D 571     138.011   0.726  58.447  1.00 30.11      D
```

```
ATOM   8044  OD2 ASP D 571     136.818  -0.715  59.575  1.00 29.31      D
ATOM   8045  C   ASP D 571     136.590   3.382  57.759  1.00 24.07      D
ATOM   8046  O   ASP D 571     135.917   4.303  57.281  1.00 22.39      D
ATOM   8047  N   ARG D 572     137.593   2.825  57.101  1.00 23.27      D
ATOM   8048  CA  ARG D 572     137.976   3.314  55.781  1.00 22.84      D
ATOM   8049  CB  ARG D 572     139.153   2.491  55.250  1.00 21.15      D
ATOM   8050  CG  ARG D 572     138.981   1.032  55.408  1.00 19.04      D
ATOM   8051  CD  ARG D 572     140.058   0.268  54.705  1.00 20.64      D
ATOM   8052  NE  ARG D 572     141.341   0.249  55.393  1.00 22.31      D
ATOM   8053  CZ  ARG D 572     142.293  -0.649  55.130  1.00 23.14      D
ATOM   8054  NH1 ARG D 572     142.071  -1.571  54.198  1.00 17.78      D
ATOM   8055  NH2 ARG D 572     143.449  -0.646  55.799  1.00 23.35      D
ATOM   8056  C   ARG D 572     136.820   3.300  54.789  1.00 22.51      D
ATOM   8057  O   ARG D 572     135.914   2.475  54.922  1.00 22.42      D
ATOM   8058  N   ILE D 573     136.825   4.241  53.837  1.00 23.14      D
ATOM   8059  CA  ILE D 573     135.779   4.301  52.809  1.00 24.51      D
ATOM   8060  CB  ILE D 573     135.449   5.739  52.295  1.00 27.12      D
ATOM   8061  CG2 ILE D 573     134.618   5.643  51.025  0.00 26.23      D
ATOM   8062  CG1 ILE D 573     134.652   6.536  53.333  1.00 26.27      D
ATOM   8063  CD1 ILE D 573     135.472   7.060  54.419  1.00 25.64      D
ATOM   8064  C   ILE D 573     136.330   3.577  51.601  1.00 24.11      D
ATOM   8065  O   ILE D 573     137.517   3.724  51.270  1.00 23.80      D
ATOM   8066  N   TYR D 574     135.459   2.830  50.927  1.00 22.78      D
ATOM   8067  CA  TYR D 574     135.849   2.071  49.742  1.00 22.23      D
ATOM   8068  CB  TYR D 574     135.498   0.583  49.951  1.00 21.98      D
ATOM   8069  CG  TYR D 574     136.588  -0.242  50.619  1.00 24.35      D
ATOM   8070  CD1 TYR D 574     137.503  -0.992  49.853  1.00 22.37      D
ATOM   8071  CE1 TYR D 574     138.524  -1.729  50.463  1.00 23.23      D
ATOM   8072  CD2 TYR D 574     136.723  -0.254  52.019  1.00 24.83      D
ATOM   8073  CE2 TYR D 574     137.736  -0.982  52.641  1.00 26.35      D
ATOM   8074  CZ  TYR D 574     138.639  -1.719  51.862  1.00 25.64      D
ATOM   8075  OH  TYR D 574     139.650  -2.423  52.493  1.00 26.87      D
ATOM   8076  C   TYR D 574     135.245   2.570  48.402  1.00 21.18      D
ATOM   8077  O   TYR D 574     135.716   2.188  47.325  1.00 22.28      D
ATOM   8078  N   SER D 575     134.231   3.432  48.464  1.00 19.10      D
ATOM   8079  CA  SER D 575     133.556   3.933  47.258  1.00 18.07      D
ATOM   8080  CB  SER D 575     132.559   2.872  46.756  1.00 18.09      D
ATOM   8081  OG  SER D 575     131.552   3.435  45.926  1.00 17.37      D
ATOM   8082  C   SER D 575     132.814   5.255  47.504  1.00 17.95      D
ATOM   8083  O   SER D 575     132.312   5.515  48.599  1.00 17.19      D
ATOM   8084  N   THR D 576     132.731   6.105  46.498  1.00 17.64      D
ATOM   8085  CA  THR D 576     132.009   7.334  46.737  1.00 19.01      D
ATOM   8086  CB  THR D 576     132.936   8.441  47.285  1.00 17.27      D
ATOM   8087  OG1 THR D 576     132.145   9.575  47.662  1.00 15.53      D
ATOM   8088  CG2 THR D 576     133.968   8.869  46.228  1.00 20.28      D
ATOM   8089  C   THR D 576     131.369   7.808  45.454  1.00 19.84      D
ATOM   8090  O   THR D 576     131.878   7.565  44.358  1.00 20.54      D
ATOM   8091  N   ILE D 577     130.228   8.461  45.571  1.00 18.92      D
ATOM   8092  CA  ILE D 577     129.622   8.959  44.366  1.00 20.24      D
ATOM   8093  CB  ILE D 577     128.395   8.161  43.984  1.00 19.47      D
ATOM   8094  CG2 ILE D 577     127.588   8.938  42.958  1.00 17.51      D
ATOM   8095  CG1 ILE D 577     128.818   6.790  43.456  1.00 19.93      D
ATOM   8096  CD1 ILE D 577     127.641   5.922  43.008  1.00 20.62      D
ATOM   8097  C   ILE D 577     129.232  10.403  44.528  1.00 21.53      D
```

```
ATOM   8098  O   ILE D 577     128.603  10.777  45.530  1.00 23.56      D
ATOM   8099  N   TYR D 578     129.615  11.223  43.551  1.00 20.82      D
ATOM   8100  CA  TYR D 578     129.264  12.644  43.593  1.00 21.04      D
ATOM   8101  CB  TYR D 578     130.384  13.509  42.982  1.00 21.65      D
ATOM   8102  CG  TYR D 578     130.022  14.975  42.792  1.00 22.52      D
ATOM   8103  CD1 TYR D 578     129.168  15.625  43.690  1.00 22.16      D
ATOM   8104  CE1 TYR D 578     128.795  16.960  43.506  1.00 21.60      D
ATOM   8105  CD2 TYR D 578     130.510  15.702  41.701  1.00 21.12      D
ATOM   8106  CE2 TYR D 578     130.147  17.038  41.506  1.00 21.36      D
ATOM   8107  CZ  TYR D 578     129.286  17.663  42.410  1.00 21.53      D
ATOM   8108  OH  TYR D 578     128.900  18.977  42.212  1.00 21.71      D
ATOM   8109  C   TYR D 578     127.955  12.883  42.851  1.00 20.91      D
ATOM   8110  O   TYR D 578     127.939  12.885  41.633  1.00 21.83      D
ATOM   8111  N   ASP D 579     126.866  13.094  43.596  1.00 22.68      D
ATOM   8112  CA  ASP D 579     125.534  13.342  43.017  1.00 24.76      D
ATOM   8113  CB  ASP D 579     124.440  13.037  44.054  1.00 25.04      D
ATOM   8114  CG  ASP D 579     123.029  12.930  43.443  1.00 27.17      D
ATOM   8115  OD1 ASP D 579     122.790  13.506  42.363  1.00 26.43      D
ATOM   8116  OD2 ASP D 579     122.144  12.271  44.061  1.00 27.38      D
ATOM   8117  C   ASP D 579     125.435  14.808  42.583  1.00 26.38      D
ATOM   8118  O   ASP D 579     124.715  15.590  43.200  1.00 25.82      D
ATOM   8119  N   HIS D 580     126.148  15.172  41.513  1.00 28.39      D
ATOM   8120  CA  HIS D 580     126.145  16.555  41.028  1.00 31.78      D
ATOM   8121  CB  HIS D 580     127.029  16.692  39.794  1.00 33.03      D
ATOM   8122  CG  HIS D 580     126.607  15.830  38.654  1.00 37.41      D
ATOM   8123  CD2 HIS D 580     125.611  15.973  37.750  1.00 38.10      D
ATOM   8124  ND1 HIS D 580     127.244  14.648  38.342  1.00 39.09      D
ATOM   8125  CE1 HIS D 580     126.660  14.102  37.292  1.00 38.85      D
ATOM   8126  NE2 HIS D 580     125.666  14.885  36.913  1.00 39.22      D
ATOM   8127  C   HIS D 580     124.745  17.113  40.723  1.00 33.01      D
ATOM   8128  O   HIS D 580     124.484  18.313  40.890  1.00 34.71      D
ATOM   8129  N   GLU D 581     123.836  16.251  40.292  1.00 33.24      D
ATOM   8130  CA  GLU D 581     122.486  16.693  39.995  1.00 32.71      D
ATOM   8131  CB  GLU D 581     121.700  15.544  39.375  1.00 35.03      D
ATOM   8132  CG  GLU D 581     120.463  15.978  38.652  1.00 39.07      D
ATOM   8133  CD  GLU D 581     119.702  14.818  38.092  1.00 41.55      D
ATOM   8134  OE1 GLU D 581     120.332  14.026  37.350  1.00 43.80      D
ATOM   8135  OE2 GLU D 581     118.485  14.712  38.394  1.00 41.52      D
ATOM   8136  C   GLU D 581     121.788  17.202  41.266  1.00 31.80      D
ATOM   8137  O   GLU D 581     121.244  18.306  41.260  1.00 31.97      D
ATOM   8138  N   ARG D 582     121.808  16.414  42.348  1.00 29.57      D
ATOM   8139  CA  ARG D 582     121.177  16.825  43.616  1.00 29.36      D
ATOM   8140  CB  ARG D 582     120.622  15.607  44.390  1.00 26.09      D
ATOM   8141  CG  ARG D 582     119.558  14.822  43.650  1.00 22.04      D
ATOM   8142  CD  ARG D 582     118.850  13.766  44.496  1.00 20.11      D
ATOM   8143  NE  ARG D 582     118.024  12.908  43.636  1.00 19.38      D
ATOM   8144  CZ  ARG D 582     118.506  12.137  42.658  1.00 20.74      D
ATOM   8145  NH1 ARG D 582     119.808  12.105  42.415  1.00 22.11      D
ATOM   8146  NH2 ARG D 582     117.695  11.398  41.908  1.00 19.51      D
ATOM   8147  C   ARG D 582     122.160  17.598  44.531  1.00 31.40      D
ATOM   8148  O   ARG D 582     121.796  18.063  45.622  1.00 29.69      D
ATOM   8149  N   LYS D 583     123.401  17.747  44.074  1.00 33.89      D
ATOM   8150  CA  LYS D 583     124.433  18.436  44.849  1.00 35.05      D
ATOM   8151  CB  LYS D 583     124.069  19.912  45.068  1.00 38.08      D
```

```
ATOM   8152  CG  LYS D 583     124.348  20.830  43.882  1.00 40.35      D
ATOM   8153  CD  LYS D 583     125.842  20.963  43.611  1.00 42.80      D
ATOM   8154  CE  LYS D 583     126.103  21.734  42.310  1.00 42.80      D
ATOM   8155  NZ  LYS D 583     125.618  23.153  42.366  1.00 43.25      D
ATOM   8156  C   LYS D 583     124.627  17.755  46.202  1.00 34.05      D
ATOM   8157  O   LYS D 583     124.524  18.401  47.241  1.00 35.02      D
ATOM   8158  N   ARG D 584     124.898  16.449  46.172  1.00 33.23      D
ATOM   8159  CA  ARG D 584     125.128  15.634  47.370  1.00 31.46      D
ATOM   8160  CB  ARG D 584     123.854  14.861  47.768  1.00 29.44      D
ATOM   8161  CG  ARG D 584     122.595  15.702  47.938  1.00 30.45      D
ATOM   8162  CD  ARG D 584     121.369  14.815  48.175  1.00 30.86      D
ATOM   8163  NE  ARG D 584     120.098  15.542  48.113  1.00 31.46      D
ATOM   8164  CZ  ARG D 584     118.904  14.965  48.229  1.00 32.25      D
ATOM   8165  NH1 ARG D 584     118.820  13.653  48.414  1.00 29.52      D
ATOM   8166  NH2 ARG D 584     117.793  15.697  48.156  1.00 30.64      D
ATOM   8167  C   ARG D 584     126.247  14.622  47.065  1.00 31.14      D
ATOM   8168  O   ARG D 584     126.668  14.466  45.916  1.00 30.87      D
ATOM   8169  N   CYS D 585     126.732  13.961  48.111  1.00 30.50      D
ATOM   8170  CA  CYS D 585     127.762  12.937  48.009  1.00 29.49      D
ATOM   8171  CB  CYS D 585     129.086  13.427  48.598  1.00 32.51      D
ATOM   8172  SG  CYS D 585     130.268  12.081  49.098  1.00 36.50      D
ATOM   8173  C   CYS D 585     127.298  11.719  48.809  1.00 28.24      D
ATOM   8174  O   CYS D 585     126.814  11.850  49.943  1.00 28.12      D
ATOM   8175  N   ILE D 586     127.434  10.546  48.193  1.00 25.25      D
ATOM   8176  CA  ILE D 586     127.094   9.266  48.806  1.00 22.27      D
ATOM   8177  CB  ILE D 586     126.394   8.304  47.804  1.00 21.75      D
ATOM   8178  CG2 ILE D 586     126.164   6.967  48.464  1.00 18.50      D
ATOM   8179  CG1 ILE D 586     125.070   8.900  47.279  1.00 21.75      D
ATOM   8180  CD1 ILE D 586     125.217   9.902  46.122  1.00 19.83      D
ATOM   8181  C   ILE D 586     128.460   8.670  49.123  1.00 22.41      D
ATOM   8182  O   ILE D 586     129.400   8.875  48.359  1.00 24.24      D
ATOM   8183  N   SER D 587     128.586   7.955  50.236  1.00 21.77      D
ATOM   8184  CA  SER D 587     129.856   7.319  50.595  1.00 19.65      D
ATOM   8185  CB  SER D 587     130.644   8.217  51.548  1.00 18.81      D
ATOM   8186  OG  SER D 587     129.942   8.436  52.758  1.00 17.09      D
ATOM   8187  C   SER D 587     129.579   5.968  51.255  1.00 19.73      D
ATOM   8188  O   SER D 587     128.676   5.867  52.082  1.00 20.77      D
ATOM   8189  N   ALA D 588     130.334   4.936  50.874  1.00 19.14      D
ATOM   8190  CA  ALA D 588     130.169   3.595  51.436  1.00 18.83      D
ATOM   8191  CB  ALA D 588     129.817   2.586  50.342  1.00 17.57      D
ATOM   8192  C   ALA D 588     131.483   3.220  52.105  1.00 18.48      D
ATOM   8193  O   ALA D 588     132.549   3.280  51.482  1.00 18.12      D
ATOM   8194  N   SER D 589     131.387   2.829  53.375  1.00 19.29      D
ATOM   8195  CA  SER D 589     132.546   2.500  54.224  1.00 20.33      D
ATOM   8196  CB  SER D 589     132.552   3.487  55.416  1.00 21.31      D
ATOM   8197  OG  SER D 589     133.427   3.106  56.474  1.00 19.54      D
ATOM   8198  C   SER D 589     132.633   1.058  54.749  1.00 20.03      D
ATOM   8199  O   SER D 589     131.638   0.322  54.743  1.00 20.59      D
ATOM   8200  N   MSE D 590     133.837   0.677  55.189  1.00 22.56      D
ATOM   8201  CA  MSE D 590     134.089  -0.644  55.760  1.00 25.48      D
ATOM   8202  CB  MSE D 590     135.578  -0.827  56.067  1.00 28.07      D
ATOM   8203  CG  MSE D 590     135.932  -2.225  56.531  1.00 30.40      D
ATOM   8204  SE  MSE D 590     137.843  -2.501  56.672  1.00 39.74      D
ATOM   8205  CE  MSE D 590     138.123  -3.610  55.120  1.00 33.01      D
```

```
ATOM   8206  C   MSE D 590     133.271  -0.777  57.053  1.00 26.26      D
ATOM   8207  O   MSE D 590     133.045  -1.883  57.540  1.00 27.96      D
ATOM   8208  N   ASP D 591     132.806   0.352  57.587  1.00 24.74      D
ATOM   8209  CA  ASP D 591     131.999   0.333  58.790  1.00 24.47      D
ATOM   8210  CB  ASP D 591     131.931   1.722  59.447  1.00 25.09      D
ATOM   8211  CG  ASP D 591     131.115   2.730  58.635  1.00 26.02      D
ATOM   8212  OD1 ASP D 591     130.116   2.338  57.987  1.00 23.16      D
ATOM   8213  OD2 ASP D 591     131.461   3.930  58.668  1.00 28.61      D
ATOM   8214  C   ASP D 591     130.575  -0.167  58.535  1.00 25.63      D
ATOM   8215  O   ASP D 591     129.731  -0.111  59.435  1.00 27.48      D
ATOM   8216  N   THR D 592     130.280  -0.612  57.315  1.00 24.13      D
ATOM   8217  CA  THR D 592     128.953  -1.144  57.027  1.00 23.60      D
ATOM   8218  CB  THR D 592     128.479  -2.010  58.217  1.00 23.93      D
ATOM   8219  OG1 THR D 592     129.276  -3.197  58.290  1.00 24.58      D
ATOM   8220  CG2 THR D 592     127.032  -2.388  58.071  1.00 25.94      D
ATOM   8221  C   THR D 592     127.858  -0.117  56.694  1.00 23.10      D
ATOM   8222  O   THR D 592     126.814  -0.466  56.131  1.00 23.01      D
ATOM   8223  N   THR D 593     128.086   1.146  57.020  1.00 21.17      D
ATOM   8224  CA  THR D 593     127.084   2.164  56.743  1.00 20.07      D
ATOM   8225  CB  THR D 593     127.097   3.238  57.829  1.00 19.96      D
ATOM   8226  OG1 THR D 593     128.317   3.981  57.736  1.00 20.19      D
ATOM   8227  CG2 THR D 593     127.012   2.601  59.205  1.00 20.49      D
ATOM   8228  C   THR D 593     127.303   2.861  55.400  1.00 20.54      D
ATOM   8229  O   THR D 593     128.282   2.602  54.705  1.00 20.50      D
ATOM   8230  N   ILE D 594     126.360   3.728  55.039  1.00 19.85      D
ATOM   8231  CA  ILE D 594     126.422   4.520  53.823  1.00 18.48      D
ATOM   8232  CB  ILE D 594     125.423   4.012  52.749  1.00 17.96      D
ATOM   8233  CG2 ILE D 594     125.476   4.931  51.512  1.00 16.27      D
ATOM   8234  CG1 ILE D 594     125.763   2.564  52.352  1.00 17.94      D
ATOM   8235  CD1 ILE D 594     124.874   1.976  51.244  1.00 13.75      D
ATOM   8236  C   ILE D 594     126.013   5.920  54.297  1.00 20.05      D
ATOM   8237  O   ILE D 594     125.125   6.060  55.147  1.00 19.44      D
ATOM   8238  N   ARG D 595     126.661   6.961  53.787  1.00 21.73      D
ATOM   8239  CA  ARG D 595     126.294   8.304  54.229  1.00 24.25      D
ATOM   8240  CB  ARG D 595     127.380   8.898  55.133  1.00 26.38      D
ATOM   8241  CG  ARG D 595     127.485   8.261  56.508  1.00 27.19      D
ATOM   8242  CD  ARG D 595     128.489   9.003  57.373  1.00 29.27      D
ATOM   8243  NE  ARG D 595     128.184   8.848  58.797  1.00 33.82      D
ATOM   8244  CZ  ARG D 595     128.465   9.753  59.732  1.00 34.00      D
ATOM   8245  NH1 ARG D 595     129.068  10.889  59.398  1.00 34.40      D
ATOM   8246  NH2 ARG D 595     128.125   9.528  60.998  1.00 33.02      D
ATOM   8247  C   ARG D 595     125.999   9.282  53.108  1.00 24.90      D
ATOM   8248  O   ARG D 595     126.702   9.329  52.102  1.00 25.43      D
ATOM   8249  N   ILE D 596     124.939  10.056  53.294  1.00 25.81      D
ATOM   8250  CA  ILE D 596     124.540  11.056  52.319  1.00 27.39      D
ATOM   8251  CB  ILE D 596     123.000  11.093  52.138  1.00 27.40      D
ATOM   8252  CG2 ILE D 596     122.646  11.950  50.935  1.00 27.77      D
ATOM   8253  CG1 ILE D 596     122.459   9.681  51.891  1.00 27.13      D
ATOM   8254  CD1 ILE D 596     122.953   9.062  50.590  1.00 26.64      D
ATOM   8255  C   ILE D 596     125.013  12.392  52.870  1.00 28.16      D
ATOM   8256  O   ILE D 596     124.637  12.787  53.976  1.00 28.61      D
ATOM   8257  N   TRP D 597     125.862  13.078  52.118  1.00 28.67      D
ATOM   8258  CA  TRP D 597     126.368  14.368  52.568  1.00 28.04      D
ATOM   8259  CB  TRP D 597     127.893  14.391  52.515  1.00 29.61      D
```

```
ATOM   8260  CG  TRP D 597     128.562  13.228  53.155  1.00 28.57      D
ATOM   8261  CD2 TRP D 597     129.116  13.186  54.470  1.00 27.43      D
ATOM   8262  CE2 TRP D 597     129.707  11.918  54.634  1.00 27.37      D
ATOM   8263  CE3 TRP D 597     129.172  14.103  55.529  1.00 27.46      D
ATOM   8264  CD1 TRP D 597     128.822  12.016  52.589  1.00 29.00      D
ATOM   8265  NE1 TRP D 597     129.516  11.221  53.469  1.00 27.32      D
ATOM   8266  CZ2 TRP D 597     130.349  11.541  55.817  1.00 27.76      D
ATOM   8267  CZ3 TRP D 597     129.810  13.729  56.703  1.00 27.02      D
ATOM   8268  CH2 TRP D 597     130.389  12.457  56.838  1.00 27.58      D
ATOM   8269  C   TRP D 597     125.838  15.486  51.684  1.00 27.75      D
ATOM   8270  O   TRP D 597     125.729  15.326  50.472  1.00 27.73      D
ATOM   8271  N   ASP D 598     125.519  16.624  52.284  1.00 28.69      D
ATOM   8272  CA  ASP D 598     125.012  17.773  51.527  1.00 29.82      D
ATOM   8273  CB  ASP D 598     123.966  18.511  52.381  1.00 29.96      D
ATOM   8274  CG  ASP D 598     123.483  19.816  51.749  1.00 30.01      D
ATOM   8275  OD1 ASP D 598     123.889  20.118  50.601  1.00 29.40      D
ATOM   8276  OD2 ASP D 598     122.700  20.537  52.417  1.00 28.15      D
ATOM   8277  C   ASP D 598     126.197  18.694  51.177  1.00 28.75      D
ATOM   8278  O   ASP D 598     126.880  19.192  52.067  1.00 26.58      D
ATOM   8279  N   LEU D 599     126.442  18.912  49.884  1.00 29.62      D
ATOM   8280  CA  LEU D 599     127.567  19.753  49.466  1.00 32.72      D
ATOM   8281  CB  LEU D 599     128.148  19.244  48.141  1.00 30.82      D
ATOM   8282  CG  LEU D 599     128.646  17.780  48.141  1.00 31.03      D
ATOM   8283  CD1 LEU D 599     129.360  17.472  46.822  1.00 29.75      D
ATOM   8284  CD2 LEU D 599     129.579  17.529  49.309  1.00 28.77      D
ATOM   8285  C   LEU D 599     127.238  21.246  49.383  1.00 35.04      D
ATOM   8286  O   LEU D 599     127.899  22.009  48.686  1.00 34.05      D
ATOM   8287  N   GLU D 600     126.228  21.651  50.145  1.00 39.89      D
ATOM   8288  CA  GLU D 600     125.793  23.041  50.205  1.00 42.71      D
ATOM   8289  CB  GLU D 600     124.279  23.118  49.998  1.00 43.83      D
ATOM   8290  CG  GLU D 600     123.818  22.578  48.659  1.00 49.15      D
ATOM   8291  CD  GLU D 600     124.057  23.565  47.524  1.00 52.47      D
ATOM   8292  OE1 GLU D 600     123.836  23.205  46.340  1.00 54.37      D
ATOM   8293  OE2 GLU D 600     124.462  24.710  47.820  1.00 53.81      D
ATOM   8294  C   GLU D 600     126.154  23.614  51.581  1.00 43.08      D
ATOM   8295  O   GLU D 600     125.956  24.799  51.847  1.00 44.92      D
ATOM   8296  N   ASN D 605     126.681  22.769  52.461  1.00 42.60      D
ATOM   8297  CA  ASN D 605     127.049  23.217  53.798  1.00 41.25      D
ATOM   8298  CB  ASN D 605     125.787  23.392  54.640  1.00 41.21      D
ATOM   8299  CG  ASN D 605     125.003  22.105  54.794  1.00 42.82      D
ATOM   8300  OD1 ASN D 605     124.753  21.383  53.830  1.00 41.44      D
ATOM   8301  ND2 ASN D 605     124.599  21.819  56.024  1.00 44.97      D
ATOM   8302  C   ASN D 605     128.006  22.222  54.440  1.00 40.16      D
ATOM   8303  O   ASN D 605     128.507  22.442  55.544  1.00 39.89      D
ATOM   8304  N   GLY D 606     128.259  21.135  53.712  1.00 39.38      D
ATOM   8305  CA  GLY D 606     129.165  20.091  54.156  1.00 36.83      D
ATOM   8306  C   GLY D 606     128.629  19.279  55.311  1.00 35.89      D
ATOM   8307  O   GLY D 606     129.336  18.446  55.865  1.00 35.05      D
ATOM   8308  N   GLU D 607     127.378  19.523  55.675  1.00 35.04      D
ATOM   8309  CA  GLU D 607     126.771  18.814  56.779  1.00 35.34      D
ATOM   8310  CB  GLU D 607     125.624  19.635  57.350  1.00 38.59      D
ATOM   8311  CG  GLU D 607     126.032  20.652  58.401  1.00 44.13      D
ATOM   8312  CD  GLU D 607     124.828  21.150  59.183  1.00 49.69      D
ATOM   8313  OE1 GLU D 607     124.093  20.289  59.749  1.00 51.01      D
```

```
ATOM   8314  OE2 GLU D 607     124.608  22.394  59.227  1.00 52.33      D
ATOM   8315  C   GLU D 607     126.271  17.415  56.411  1.00 33.71      D
ATOM   8316  O   GLU D 607     125.991  17.144  55.247  1.00 33.25      D
ATOM   8317  N   LEU D 608     126.175  16.521  57.397  1.00 31.85      D
ATOM   8318  CA  LEU D 608     125.686  15.175  57.125  1.00 30.51      D
ATOM   8319  CB  LEU D 608     126.052  14.216  58.253  1.00 27.96      D
ATOM   8320  CG  LEU D 608     125.557  12.778  58.041  1.00 28.56      D
ATOM   8321  CD1 LEU D 608     126.456  12.051  57.046  1.00 24.69      D
ATOM   8322  CD2 LEU D 608     125.531  12.032  59.394  1.00 28.82      D
ATOM   8323  C   LEU D 608     124.169  15.253  56.971  1.00 30.57      D
ATOM   8324  O   LEU D 608     123.532  16.124  57.573  1.00 31.18      D
ATOM   8325  N   MSE D 625     123.605  14.363  56.150  1.00 29.87      D
ATOM   8326  CA  MSE D 625     122.153  14.303  55.888  1.00 30.31      D
ATOM   8327  CB  MSE D 625     121.846  14.367  54.381  1.00 31.08      D
ATOM   8328  CG  MSE D 625     122.016  15.737  53.754  1.00 33.02      D
ATOM   8329  SE  MSE D 625     121.598  15.802  51.862  1.00 38.72      D
ATOM   8330  CE  MSE D 625     119.705  15.354  51.962  1.00 32.55      D
ATOM   8331  C   MSE D 625     121.523  13.022  56.410  1.00 27.88      D
ATOM   8332  O   MSE D 625     120.538  13.032  57.145  1.00 28.06      D
ATOM   8333  N   TYR D 626     122.073  11.901  55.993  1.00 25.99      D
ATOM   8334  CA  TYR D 626     121.505  10.670  56.444  1.00 24.99      D
ATOM   8335  CB  TYR D 626     120.453  10.176  55.461  1.00 25.25      D
ATOM   8336  CG  TYR D 626     119.434  11.186  54.999  1.00 24.62      D
ATOM   8337  CD1 TYR D 626     118.409  11.612  55.842  1.00 21.86      D
ATOM   8338  CE1 TYR D 626     117.391  12.424  55.363  1.00 23.49      D
ATOM   8339  CD2 TYR D 626     119.426  11.615  53.669  1.00 24.69      D
ATOM   8340  CE2 TYR D 626     118.421  12.421  53.179  1.00 24.51      D
ATOM   8341  CZ  TYR D 626     117.396  12.820  54.023  1.00 24.72      D
ATOM   8342  OH  TYR D 626     116.346  13.555  53.502  1.00 25.76      D
ATOM   8343  C   TYR D 626     122.555   9.597  56.565  1.00 23.88      D
ATOM   8344  O   TYR D 626     123.605   9.652  55.923  1.00 23.89      D
ATOM   8345  N   THR D 627     122.255   8.616  57.406  1.00 23.42      D
ATOM   8346  CA  THR D 627     123.122   7.472  57.564  1.00 20.62      D
ATOM   8347  CB  THR D 627     123.589   7.271  58.987  1.00 19.43      D
ATOM   8348  OG1 THR D 627     124.268   8.447  59.440  1.00 20.14      D
ATOM   8349  CG2 THR D 627     124.535   6.066  59.050  1.00 17.31      D
ATOM   8350  C   THR D 627     122.235   6.308  57.191  1.00 19.41      D
ATOM   8351  O   THR D 627     121.244   6.050  57.859  1.00 18.63      D
ATOM   8352  N   LEU D 628     122.577   5.640  56.095  1.00 19.47      D
ATOM   8353  CA  LEU D 628     121.821   4.485  55.626  1.00 19.11      D
ATOM   8354  CB  LEU D 628     121.755   4.469  54.108  1.00 17.80      D
ATOM   8355  CG  LEU D 628     121.117   5.669  53.396  1.00 16.59      D
ATOM   8356  CD1 LEU D 628     121.092   5.364  51.890  1.00 16.34      D
ATOM   8357  CD2 LEU D 628     119.712   5.929  53.916  1.00 13.86      D
ATOM   8358  C   LEU D 628     122.523   3.227  56.111  1.00 19.57      D
ATOM   8359  O   LEU D 628     123.674   2.966  55.744  1.00 20.61      D
ATOM   8360  N   GLN D 629     121.817   2.456  56.936  1.00 19.21      D
ATOM   8361  CA  GLN D 629     122.331   1.216  57.512  1.00 19.59      D
ATOM   8362  CB  GLN D 629     122.142   1.262  59.031  1.00 18.99      D
ATOM   8363  CG  GLN D 629     122.640   0.047  59.795  1.00 19.95      D
ATOM   8364  CD  GLN D 629     124.155  -0.088  59.756  1.00 21.73      D
ATOM   8365  OE1 GLN D 629     124.709  -0.697  58.841  1.00 21.66      D
ATOM   8366  NE2 GLN D 629     124.834   0.492  60.751  1.00 21.48      D
ATOM   8367  C   GLN D 629     121.565   0.034  56.922  1.00 19.26      D
```

```
ATOM   8368  O   GLN D 629     120.435  -0.224  57.313  1.00 22.24      D
ATOM   8369  N   GLY D 630     122.178  -0.689  55.993  1.00 18.64      D
ATOM   8370  CA  GLY D 630     121.480  -1.802  55.386  1.00 19.70      D
ATOM   8371  C   GLY D 630     122.361  -2.917  54.860  1.00 21.44      D
ATOM   8372  O   GLY D 630     122.068  -3.533  53.844  1.00 22.81      D
ATOM   8373  N   HIS D 631     123.459  -3.179  55.544  1.00 22.39      D
ATOM   8374  CA  HIS D 631     124.368  -4.236  55.143  1.00 23.12      D
ATOM   8375  CB  HIS D 631     125.425  -3.720  54.169  1.00 26.25      D
ATOM   8376  CG  HIS D 631     124.856  -3.144  52.915  1.00 28.65      D
ATOM   8377  CD2 HIS D 631     124.544  -1.870  52.586  1.00 28.78      D
ATOM   8378  ND1 HIS D 631     124.504  -3.920  51.833  1.00 29.43      D
ATOM   8379  CE1 HIS D 631     124.002  -3.146  50.887  1.00 28.34      D
ATOM   8380  NE2 HIS D 631     124.015  -1.898  51.319  1.00 28.49      D
ATOM   8381  C   HIS D 631     125.030  -4.618  56.440  1.00 22.81      D
ATOM   8382  O   HIS D 631     125.008  -3.860  57.402  1.00 25.35      D
ATOM   8383  N   THR D 632     125.661  -5.774  56.455  1.00 21.41      D
ATOM   8384  CA  THR D 632     126.288  -6.261  57.663  1.00 20.28      D
ATOM   8385  CB  THR D 632     125.646  -7.591  58.047  1.00 18.49      D
ATOM   8386  OG1 THR D 632     125.767  -8.524  56.957  1.00 18.30      D
ATOM   8387  CG2 THR D 632     124.173  -7.371  58.349  1.00 13.99      D
ATOM   8388  C   THR D 632     127.771  -6.466  57.509  1.00 20.33      D
ATOM   8389  O   THR D 632     128.427  -6.983  58.405  1.00 22.76      D
ATOM   8390  N   ALA D 633     128.291  -6.053  56.367  1.00 19.78      D
ATOM   8391  CA  ALA D 633     129.695  -6.224  56.061  1.00 18.83      D
ATOM   8392  CB  ALA D 633     129.877  -7.469  55.239  1.00 17.26      D
ATOM   8393  C   ALA D 633     130.169  -5.029  55.282  1.00 19.55      D
ATOM   8394  O   ALA D 633     129.385  -4.126  54.991  1.00 19.68      D
ATOM   8395  N   LEU D 634     131.455  -5.024  54.951  1.00 20.72      D
ATOM   8396  CA  LEU D 634     132.051  -3.944  54.175  1.00 20.81      D
ATOM   8397  CB  LEU D 634     133.478  -4.347  53.790  1.00 21.47      D
ATOM   8398  CG  LEU D 634     134.286  -3.752  52.639  1.00 22.59      D
ATOM   8399  CD1 LEU D 634     133.982  -4.534  51.395  1.00 25.22      D
ATOM   8400  CD2 LEU D 634     133.968  -2.263  52.448  1.00 26.73      D
ATOM   8401  C   LEU D 634     131.211  -3.634  52.940  1.00 21.70      D
ATOM   8402  O   LEU D 634     130.889  -4.523  52.138  1.00 22.37      D
ATOM   8403  N   VAL D 635     130.822  -2.371  52.807  1.00 21.89      D
ATOM   8404  CA  VAL D 635     130.038  -1.957  51.646  1.00 23.38      D
ATOM   8405  CB  VAL D 635     128.929  -0.951  52.019  1.00 23.26      D
ATOM   8406  CG1 VAL D 635     128.136  -0.574  50.771  1.00 25.04      D
ATOM   8407  CG2 VAL D 635     128.008  -1.545  53.048  1.00 21.55      D
ATOM   8408  C   VAL D 635     131.019  -1.303  50.670  1.00 24.61      D
ATOM   8409  O   VAL D 635     131.455  -0.164  50.878  1.00 22.67      D
ATOM   8410  N   GLY D 636     131.352  -2.036  49.607  1.00 25.64      D
ATOM   8411  CA  GLY D 636     132.320  -1.552  48.641  1.00 26.53      D
ATOM   8412  C   GLY D 636     131.874  -1.151  47.254  1.00 26.66      D
ATOM   8413  O   GLY D 636     132.687  -0.595  46.509  1.00 27.11      D
ATOM   8414  N   LEU D 637     130.612  -1.418  46.906  1.00 26.43      D
ATOM   8415  CA  LEU D 637     130.077  -1.089  45.582  1.00 24.26      D
ATOM   8416  CB  LEU D 637     129.705  -2.367  44.825  1.00 22.49      D
ATOM   8417  CG  LEU D 637     130.896  -3.277  44.542  1.00 21.34      D
ATOM   8418  CD1 LEU D 637     132.028  -2.399  44.003  1.00 18.59      D
ATOM   8419  CD2 LEU D 637     131.352  -3.982  45.809  1.00 23.19      D
ATOM   8420  C   LEU D 637     128.868  -0.163  45.606  1.00 25.18      D
ATOM   8421  O   LEU D 637     127.843  -0.503  46.182  1.00 26.31      D
```

```
ATOM   8422  N   LEU D 638     129.009   1.004  44.970  1.00 26.27      D
ATOM   8423  CA  LEU D 638     127.959   2.021  44.854  1.00 25.24      D
ATOM   8424  CB  LEU D 638     128.335   3.308  45.579  1.00 25.17      D
ATOM   8425  CG  LEU D 638     128.217   3.292  47.092  1.00 26.38      D
ATOM   8426  CD1 LEU D 638     128.445   4.708  47.617  1.00 25.29      D
ATOM   8427  CD2 LEU D 638     126.827   2.778  47.484  1.00 23.90      D
ATOM   8428  C   LEU D 638     127.772   2.372  43.396  1.00 25.47      D
ATOM   8429  O   LEU D 638     128.746   2.427  42.638  1.00 24.74      D
ATOM   8430  N   ARG D 639     126.515   2.639  43.029  1.00 25.82      D
ATOM   8431  CA  ARG D 639     126.101   2.999  41.661  1.00 24.67      D
ATOM   8432  CB  ARG D 639     125.735   1.733  40.875  1.00 24.23      D
ATOM   8433  CG  ARG D 639     126.472   1.524  39.569  1.00 24.13      D
ATOM   8434  CD  ARG D 639     127.923   1.341  39.843  1.00 24.24      D
ATOM   8435  NE  ARG D 639     128.539   0.275  39.061  1.00 25.29      D
ATOM   8436  CZ  ARG D 639     129.345   0.488  38.027  1.00 26.83      D
ATOM   8437  NH1 ARG D 639     129.609   1.735  37.658  1.00 22.95      D
ATOM   8438  NH2 ARG D 639     129.909  -0.538  37.387  1.00 27.61      D
ATOM   8439  C   ARG D 639     124.857   3.877  41.777  1.00 24.76      D
ATOM   8440  O   ARG D 639     123.942   3.540  42.519  1.00 24.70      D
ATOM   8441  N   LEU D 640     124.821   4.991  41.046  1.00 25.49      D
ATOM   8442  CA  LEU D 640     123.668   5.908  41.066  1.00 23.58      D
ATOM   8443  CB  LEU D 640     124.142   7.354  41.250  1.00 20.68      D
ATOM   8444  CG  LEU D 640     123.301   8.220  42.178  1.00 21.27      D
ATOM   8445  CD1 LEU D 640     123.483   9.698  41.849  1.00 19.99      D
ATOM   8446  CD2 LEU D 640     121.854   7.834  42.058  1.00 21.23      D
ATOM   8447  C   LEU D 640     122.888   5.800  39.753  1.00 23.09      D
ATOM   8448  O   LEU D 640     123.464   5.886  38.677  1.00 25.33      D
ATOM   8449  N   SER D 641     121.582   5.598  39.846  1.00 22.47      D
ATOM   8450  CA  SER D 641     120.741   5.498  38.668  1.00 21.80      D
ATOM   8451  CB  SER D 641     119.920   4.212  38.713  1.00 23.05      D
ATOM   8452  OG  SER D 641     118.628   4.399  38.170  1.00 26.20      D
ATOM   8453  C   SER D 641     119.837   6.712  38.706  1.00 22.79      D
ATOM   8454  O   SER D 641     119.697   7.344  39.743  1.00 21.44      D
ATOM   8455  N   ASP D 642     119.206   7.052  37.596  1.00 25.87      D
ATOM   8456  CA  ASP D 642     118.361   8.230  37.631  1.00 29.02      D
ATOM   8457  CB  ASP D 642     117.753   8.507  36.258  1.00 32.11      D
ATOM   8458  CG  ASP D 642     117.066   9.854  36.206  1.00 35.97      D
ATOM   8459  OD1 ASP D 642     117.782  10.877  36.333  1.00 38.30      D
ATOM   8460  OD2 ASP D 642     115.817   9.904  36.059  1.00 37.81      D
ATOM   8461  C   ASP D 642     117.247   8.077  38.655  1.00 28.71      D
ATOM   8462  O   ASP D 642     116.649   9.055  39.098  1.00 28.83      D
ATOM   8463  N   LYS D 643     116.975   6.847  39.047  1.00 29.24      D
ATOM   8464  CA  LYS D 643     115.903   6.626  39.989  1.00 29.96      D
ATOM   8465  CB  LYS D 643     114.760   5.934  39.241  1.00 31.36      D
ATOM   8466  CG  LYS D 643     113.626   5.382  40.076  1.00 36.57      D
ATOM   8467  CD  LYS D 643     112.491   4.792  39.183  1.00 38.95      D
ATOM   8468  CE  LYS D 643     111.899   5.844  38.222  1.00 40.27      D
ATOM   8469  NZ  LYS D 643     110.719   5.330  37.453  1.00 40.99      D
ATOM   8470  C   LYS D 643     116.325   5.831  41.222  1.00 29.02      D
ATOM   8471  O   LYS D 643     115.628   5.832  42.234  1.00 29.30      D
ATOM   8472  N   PHE D 644     117.483   5.187  41.160  1.00 27.45      D
ATOM   8473  CA  PHE D 644     117.924   4.370  42.276  1.00 25.90      D
ATOM   8474  CB  PHE D 644     117.822   2.889  41.918  1.00 23.62      D
ATOM   8475  CG  PHE D 644     116.428   2.416  41.670  1.00 22.94      D
```

ATOM	8476	CD1	PHE	D	644	116.097	1.784	40.480	1.00	23.53	D
ATOM	8477	CD2	PHE	D	644	115.448	2.567	42.632	1.00	21.03	D
ATOM	8478	CE1	PHE	D	644	114.807	1.309	40.266	1.00	21.81	D
ATOM	8479	CE2	PHE	D	644	114.164	2.094	42.416	1.00	18.29	D
ATOM	8480	CZ	PHE	D	644	113.847	1.467	41.237	1.00	17.27	D
ATOM	8481	C	PHE	D	644	119.337	4.618	42.735	1.00	26.43	D
ATOM	8482	O	PHE	D	644	120.164	5.136	41.989	1.00	25.68	D
ATOM	8483	N	LEU	D	645	119.589	4.238	43.988	1.00	27.14	D
ATOM	8484	CA	LEU	D	645	120.911	4.318	44.608	1.00	26.31	D
ATOM	8485	CB	LEU	D	645	120.914	5.234	45.828	1.00	27.08	D
ATOM	8486	CG	LEU	D	645	122.217	5.194	46.640	1.00	27.94	D
ATOM	8487	CD1	LEU	D	645	123.290	5.975	45.918	1.00	29.78	D
ATOM	8488	CD2	LEU	D	645	121.994	5.766	48.028	1.00	27.68	D
ATOM	8489	C	LEU	D	645	121.152	2.890	45.059	1.00	24.69	D
ATOM	8490	O	LEU	D	645	120.758	2.514	46.146	1.00	26.35	D
ATOM	8491	N	VAL	D	646	121.786	2.100	44.206	1.00	23.16	D
ATOM	8492	CA	VAL	D	646	122.056	0.706	44.499	1.00	21.12	D
ATOM	8493	CB	VAL	D	646	122.116	-0.101	43.212	1.00	20.50	D
ATOM	8494	CG1	VAL	D	646	122.047	-1.583	43.514	1.00	21.04	D
ATOM	8495	CG2	VAL	D	646	120.997	0.334	42.283	1.00	20.61	D
ATOM	8496	C	VAL	D	646	123.384	0.523	45.211	1.00	20.80	D
ATOM	8497	O	VAL	D	646	124.375	1.159	44.857	1.00	21.52	D
ATOM	8498	N	SER	D	647	123.408	-0.356	46.208	1.00	20.76	D
ATOM	8499	CA	SER	D	647	124.637	-0.643	46.936	1.00	19.72	D
ATOM	8500	CB	SER	D	647	124.706	0.166	48.231	1.00	19.38	D
ATOM	8501	OG	SER	D	647	123.594	-0.100	49.071	1.00	20.83	D
ATOM	8502	C	SER	D	647	124.723	-2.140	47.249	1.00	19.78	D
ATOM	8503	O	SER	D	647	123.694	-2.816	47.373	1.00	18.23	D
ATOM	8504	N	ALA	D	648	125.950	-2.654	47.344	1.00	18.94	D
ATOM	8505	CA	ALA	D	648	126.175	-4.060	47.646	1.00	19.09	D
ATOM	8506	CB	ALA	D	648	126.463	-4.850	46.377	1.00	15.72	D
ATOM	8507	C	ALA	D	648	127.337	-4.180	48.618	1.00	20.74	D
ATOM	8508	O	ALA	D	648	128.279	-3.399	48.547	1.00	22.53	D
ATOM	8509	N	ALA	D	649	127.253	-5.148	49.533	1.00	21.16	D
ATOM	8510	CA	ALA	D	649	128.301	-5.372	50.514	1.00	20.36	D
ATOM	8511	CB	ALA	D	649	127.774	-5.097	51.911	1.00	23.59	D
ATOM	8512	C	ALA	D	649	128.912	-6.772	50.457	1.00	20.64	D
ATOM	8513	O	ALA	D	649	128.453	-7.663	49.723	1.00	19.52	D
ATOM	8514	N	ALA	D	650	129.951	-6.944	51.271	1.00	18.79	D
ATOM	8515	CA	ALA	D	650	130.703	-8.192	51.372	1.00	17.83	D
ATOM	8516	CB	ALA	D	650	131.839	-8.012	52.334	1.00	17.25	D
ATOM	8517	C	ALA	D	650	129.889	-9.409	51.786	1.00	17.38	D
ATOM	8518	O	ALA	D	650	130.337	-10.545	51.626	1.00	16.75	D
ATOM	8519	N	ASP	D	651	128.699	-9.190	52.329	1.00	18.32	D
ATOM	8520	CA	ASP	D	651	127.880	-10.323	52.748	1.00	19.29	D
ATOM	8521	CB	ASP	D	651	126.982	-9.930	53.920	1.00	21.96	D
ATOM	8522	CG	ASP	D	651	126.027	-8.804	53.568	1.00	26.40	D
ATOM	8523	OD1	ASP	D	651	125.508	-8.816	52.425	1.00	28.33	D
ATOM	8524	OD2	ASP	D	651	125.781	-7.924	54.436	1.00	25.72	D
ATOM	8525	C	ASP	D	651	127.026	-10.856	51.609	1.00	19.07	D
ATOM	8526	O	ASP	D	651	126.244	-11.789	51.787	1.00	20.37	D
ATOM	8527	N	GLY	D	652	127.164	-10.256	50.437	1.00	19.11	D
ATOM	8528	CA	GLY	D	652	126.370	-10.711	49.315	1.00	18.71	D
ATOM	8529	C	GLY	D	652	125.024	-10.018	49.213	1.00	18.78	D

```
ATOM   8530  O   GLY D 652     124.142 -10.475  48.479  1.00 17.99      D
ATOM   8531  N   SER D 653     124.841  -8.926  49.950  1.00 20.24      D
ATOM   8532  CA  SER D 653     123.575  -8.198  49.864  1.00 21.58      D
ATOM   8533  CB  SER D 653     123.133  -7.678  51.236  1.00 21.54      D
ATOM   8534  OG  SER D 653     124.037  -6.731  51.772  1.00 22.98      D
ATOM   8535  C   SER D 653     123.665  -7.033  48.881  1.00 22.14      D
ATOM   8536  O   SER D 653     124.742  -6.510  48.598  1.00 21.79      D
ATOM   8537  N   ILE D 654     122.515  -6.652  48.350  1.00 23.25      D
ATOM   8538  CA  ILE D 654     122.418  -5.554  47.409  1.00 25.80      D
ATOM   8539  CB  ILE D 654     122.165  -6.055  45.982  1.00 26.21      D
ATOM   8540  CG2 ILE D 654     122.297  -4.918  45.003  1.00 26.27      D
ATOM   8541  CG1 ILE D 654     123.154  -7.158  45.616  1.00 28.16      D
ATOM   8542  CD1 ILE D 654     122.870  -7.785  44.254  1.00 28.37      D
ATOM   8543  C   ILE D 654     121.197  -4.754  47.836  1.00 26.75      D
ATOM   8544  O   ILE D 654     120.122  -5.323  48.064  1.00 27.01      D
ATOM   8545  N   ARG D 655     121.346  -3.443  47.951  1.00 27.07      D
ATOM   8546  CA  ARG D 655     120.216  -2.626  48.356  1.00 27.67      D
ATOM   8547  CB  ARG D 655     120.467  -2.029  49.737  1.00 28.04      D
ATOM   8548  CG  ARG D 655     120.592  -3.062  50.832  1.00 29.00      D
ATOM   8549  CD  ARG D 655     119.901  -2.605  52.103  1.00 31.71      D
ATOM   8550  NE  ARG D 655     118.574  -3.199  52.240  1.00 33.84      D
ATOM   8551  CZ  ARG D 655     118.328  -4.314  52.914  1.00 33.80      D
ATOM   8552  NH1 ARG D 655     119.314  -4.960  53.527  1.00 33.02      D
ATOM   8553  NH2 ARG D 655     117.094  -4.787  52.953  1.00 36.00      D
ATOM   8554  C   ARG D 655     119.903  -1.524  47.358  1.00 27.31      D
ATOM   8555  O   ARG D 655     120.797  -0.985  46.706  1.00 26.04      D
ATOM   8556  N   GLY D 656     118.620  -1.203  47.237  1.00 27.56      D
ATOM   8557  CA  GLY D 656     118.206  -0.164  46.315  1.00 28.15      D
ATOM   8558  C   GLY D 656     117.482   0.916  47.087  1.00 27.66      D
ATOM   8559  O   GLY D 656     116.514   0.621  47.775  1.00 28.41      D
ATOM   8560  N   TRP D 657     117.944   2.158  46.996  1.00 27.78      D
ATOM   8561  CA  TRP D 657     117.299   3.256  47.715  1.00 28.29      D
ATOM   8562  CB  TRP D 657     118.296   3.913  48.699  1.00 26.47      D
ATOM   8563  CG  TRP D 657     119.251   2.947  49.419  1.00 24.99      D
ATOM   8564  CD2 TRP D 657     119.136   2.448  50.768  1.00 23.38      D
ATOM   8565  CE2 TRP D 657     120.215   1.554  50.972  1.00 22.65      D
ATOM   8566  CE3 TRP D 657     118.226   2.664  51.818  1.00 22.66      D
ATOM   8567  CD1 TRP D 657     120.369   2.352  48.891  1.00 22.06      D
ATOM   8568  NE1 TRP D 657     120.947   1.520  49.815  1.00 21.92      D
ATOM   8569  CZ2 TRP D 657     120.407   0.875  52.180  1.00 20.78      D
ATOM   8570  CZ3 TRP D 657     118.423   1.979  53.026  1.00 22.09      D
ATOM   8571  CH2 TRP D 657     119.505   1.098  53.187  1.00 22.26      D
ATOM   8572  C   TRP D 657     116.777   4.313  46.705  1.00 29.51      D
ATOM   8573  O   TRP D 657     117.304   4.422  45.592  1.00 29.88      D
ATOM   8574  N   ASP D 658     115.744   5.076  47.075  1.00 29.21      D
ATOM   8575  CA  ASP D 658     115.223   6.104  46.174  1.00 29.96      D
ATOM   8576  CB  ASP D 658     113.977   6.790  46.757  1.00 28.48      D
ATOM   8577  CG  ASP D 658     113.460   7.923  45.868  1.00 28.43      D
ATOM   8578  OD1 ASP D 658     112.888   7.650  44.793  1.00 28.91      D
ATOM   8579  OD2 ASP D 658     113.628   9.101  46.236  1.00 27.59      D
ATOM   8580  C   ASP D 658     116.354   7.113  46.026  1.00 31.50      D
ATOM   8581  O   ASP D 658     116.978   7.503  47.017  1.00 32.96      D
ATOM   8582  N   ALA D 659     116.621   7.526  44.791  1.00 31.88      D
ATOM   8583  CA  ALA D 659     117.694   8.468  44.499  1.00 32.44      D
```

```
ATOM   8584  CB  ALA D 659     117.811   8.649  43.010  1.00 32.07      D
ATOM   8585  C   ALA D 659     117.541   9.829  45.162  1.00 33.56      D
ATOM   8586  O   ALA D 659     118.463  10.634  45.141  1.00 34.05      D
ATOM   8587  N   ASN D 660     116.387  10.091  45.761  1.00 36.44      D
ATOM   8588  CA  ASN D 660     116.155  11.379  46.400  1.00 37.59      D
ATOM   8589  CB  ASN D 660     115.061  12.130  45.645  1.00 39.91      D
ATOM   8590  CG  ASN D 660     114.872  13.542  46.149  1.00 43.39      D
ATOM   8591  OD1 ASN D 660     114.382  13.764  47.264  1.00 44.43      D
ATOM   8592  ND2 ASN D 660     115.274  14.515  45.334  1.00 45.95      D
ATOM   8593  C   ASN D 660     115.791  11.248  47.876  1.00 36.76      D
ATOM   8594  O   ASN D 660     116.233  12.050  48.689  1.00 38.43      D
ATOM   8595  N   ASP D 661     114.991  10.239  48.214  1.00 35.26      D
ATOM   8596  CA  ASP D 661     114.566   9.984  49.592  1.00 33.16      D
ATOM   8597  CB  ASP D 661     113.165   9.393  49.620  1.00 34.45      D
ATOM   8598  CG  ASP D 661     112.144  10.331  49.104  1.00 38.11      D
ATOM   8599  OD1 ASP D 661     112.280  11.540  49.419  1.00 40.95      D
ATOM   8600  OD2 ASP D 661     111.200   9.876  48.409  1.00 39.95      D
ATOM   8601  C   ASP D 661     115.458   8.980  50.292  1.00 31.13      D
ATOM   8602  O   ASP D 661     115.569   9.004  51.505  1.00 31.79      D
ATOM   8603  N   TYR D 662     116.023   8.062  49.517  1.00 26.92      D
ATOM   8604  CA  TYR D 662     116.885   7.016  50.027  1.00 25.03      D
ATOM   8605  CB  TYR D 662     118.028   7.615  50.876  1.00 23.52      D
ATOM   8606  CG  TYR D 662     118.839   8.622  50.075  1.00 24.99      D
ATOM   8607  CD1 TYR D 662     119.614   8.201  48.999  1.00 23.45      D
ATOM   8608  CE1 TYR D 662     120.257   9.099  48.181  1.00 23.80      D
ATOM   8609  CD2 TYR D 662     118.739   9.996  50.317  1.00 23.15      D
ATOM   8610  CE2 TYR D 662     119.384  10.914  49.497  1.00 24.08      D
ATOM   8611  CZ  TYR D 662     120.143  10.459  48.424  1.00 25.80      D
ATOM   8612  OH  TYR D 662     120.770  11.367  47.581  1.00 25.60      D
ATOM   8613  C   TYR D 662     116.090   5.979  50.808  1.00 24.80      D
ATOM   8614  O   TYR D 662     116.663   5.210  51.590  1.00 25.89      D
ATOM   8615  N   SER D 663     114.777   5.946  50.575  1.00 21.66      D
ATOM   8616  CA  SER D 663     113.886   4.981  51.228  1.00 21.07      D
ATOM   8617  CB  SER D 663     112.432   5.460  51.165  1.00 20.52      D
ATOM   8618  OG  SER D 663     111.987   5.642  49.838  1.00 19.13      D
ATOM   8619  C   SER D 663     113.996   3.610  50.564  1.00 20.63      D
ATOM   8620  O   SER D 663     114.182   3.530  49.357  1.00 20.77      D
ATOM   8621  N   ARG D 664     113.901   2.537  51.353  1.00 21.12      D
ATOM   8622  CA  ARG D 664     114.022   1.180  50.819  1.00 20.22      D
ATOM   8623  CB  ARG D 664     113.564   0.125  51.849  1.00 22.66      D
ATOM   8624  CG  ARG D 664     114.575  -0.302  52.980  1.00 25.13      D
ATOM   8625  CD  ARG D 664     114.860   0.821  53.987  1.00 27.71      D
ATOM   8626  NE  ARG D 664     115.573   0.440  55.219  1.00 29.68      D
ATOM   8627  CZ  ARG D 664     116.626  -0.373  55.291  1.00 31.69      D
ATOM   8628  NH1 ARG D 664     117.114  -0.935  54.200  1.00 34.72      D
ATOM   8629  NH2 ARG D 664     117.226  -0.597  56.456  1.00 30.46      D
ATOM   8630  C   ARG D 664     113.196   1.037  49.552  1.00 18.91      D
ATOM   8631  O   ARG D 664     112.013   1.393  49.525  1.00 19.59      D
ATOM   8632  N   LYS D 665     113.833   0.544  48.496  1.00 17.43      D
ATOM   8633  CA  LYS D 665     113.144   0.320  47.238  1.00 16.40      D
ATOM   8634  CB  LYS D 665     113.729   1.204  46.148  1.00 14.06      D
ATOM   8635  CG  LYS D 665     113.132   2.582  46.190  1.00 13.78      D
ATOM   8636  CD  LYS D 665     111.661   2.434  45.960  1.00 14.84      D
ATOM   8637  CE  LYS D 665     110.875   3.713  46.115  1.00 14.42      D
```

```
ATOM   8638  NZ  LYS D 665     109.447   3.311  45.873  1.00 17.38      D
ATOM   8639  C   LYS D 665     113.202  -1.149  46.868  1.00 15.50      D
ATOM   8640  O   LYS D 665     112.216  -1.709  46.413  1.00 18.21      D
ATOM   8641  N   PHE D 666     114.352  -1.778  47.069  1.00 15.94      D
ATOM   8642  CA  PHE D 666     114.492  -3.207  46.810  1.00 16.38      D
ATOM   8643  CB  PHE D 666     114.453  -3.531  45.291  1.00 12.81      D
ATOM   8644  CG  PHE D 666     115.613  -2.980  44.477  1.00 13.72      D
ATOM   8645  CD1 PHE D 666     116.914  -3.428  44.676  1.00 14.32      D
ATOM   8646  CD2 PHE D 666     115.386  -2.051  43.460  1.00 16.32      D
ATOM   8647  CE1 PHE D 666     117.963  -2.962  43.881  1.00 12.43      D
ATOM   8648  CE2 PHE D 666     116.433  -1.579  42.659  1.00 14.70      D
ATOM   8649  CZ  PHE D 666     117.716  -2.039  42.873  1.00 15.14      D
ATOM   8650  C   PHE D 666     115.764  -3.767  47.482  1.00 17.88      D
ATOM   8651  O   PHE D 666     116.618  -3.017  47.971  1.00 18.62      D
ATOM   8652  N   SER D 667     115.869  -5.088  47.533  1.00 19.07      D
ATOM   8653  CA  SER D 667     117.021  -5.736  48.127  1.00 20.16      D
ATOM   8654  CB  SER D 667     116.971  -5.646  49.661  1.00 21.18      D
ATOM   8655  OG  SER D 667     115.778  -6.192  50.188  1.00 21.36      D
ATOM   8656  C   SER D 667     117.089  -7.188  47.675  1.00 19.78      D
ATOM   8657  O   SER D 667     116.093  -7.907  47.662  1.00 18.38      D
ATOM   8658  N   TYR D 668     118.280  -7.596  47.274  1.00 20.33      D
ATOM   8659  CA  TYR D 668     118.499  -8.946  46.807  1.00 21.29      D
ATOM   8660  CB  TYR D 668     118.756  -8.936  45.293  1.00 21.18      D
ATOM   8661  CG  TYR D 668     117.595  -8.369  44.470  1.00 20.55      D
ATOM   8662  CD1 TYR D 668     116.495  -9.171  44.114  1.00 18.14      D
ATOM   8663  CE1 TYR D 668     115.423  -8.647  43.403  1.00 18.24      D
ATOM   8664  CD2 TYR D 668     117.584  -7.020  44.084  1.00 18.54      D
ATOM   8665  CE2 TYR D 668     116.522  -6.484  43.379  1.00 18.25      D
ATOM   8666  CZ  TYR D 668     115.437  -7.293  43.044  1.00 19.79      D
ATOM   8667  OH  TYR D 668     114.343  -6.732  42.410  1.00 18.58      D
ATOM   8668  C   TYR D 668     119.709  -9.445  47.560  1.00 21.68      D
ATOM   8669  O   TYR D 668     120.525  -8.650  48.008  1.00 24.28      D
ATOM   8670  N   HIS D 669     119.802 -10.757  47.718  1.00 23.30      D
ATOM   8671  CA  HIS D 669     120.904 -11.398  48.413  1.00 23.12      D
ATOM   8672  CB  HIS D 669     120.433 -11.895  49.771  1.00 23.33      D
ATOM   8673  CG  HIS D 669     121.343 -11.528  50.897  1.00 26.89      D
ATOM   8674  CD2 HIS D 669     121.187 -10.654  51.921  1.00 25.28      D
ATOM   8675  ND1 HIS D 669     122.608 -12.060  51.034  1.00 26.65      D
ATOM   8676  CE1 HIS D 669     123.193 -11.529  52.093  1.00 27.24      D
ATOM   8677  NE2 HIS D 669     122.353 -10.673  52.649  1.00 27.53      D
ATOM   8678  C   HIS D 669     121.274 -12.587  47.535  1.00 24.51      D
ATOM   8679  O   HIS D 669     120.399 -13.313  47.036  1.00 24.95      D
ATOM   8680  N   HIS D 670     122.569 -12.779  47.335  1.00 24.99      D
ATOM   8681  CA  HIS D 670     123.045 -13.882  46.521  1.00 25.59      D
ATOM   8682  CB  HIS D 670     124.501 -13.642  46.121  1.00 26.37      D
ATOM   8683  CG  HIS D 670     124.666 -12.905  44.823  1.00 29.01      D
ATOM   8684  CD2 HIS D 670     125.637 -12.971  43.881  1.00 27.78      D
ATOM   8685  ND1 HIS D 670     123.779 -11.942  44.387  1.00 28.88      D
ATOM   8686  CE1 HIS D 670     124.199 -11.450  43.236  1.00 26.47      D
ATOM   8687  NE2 HIS D 670     125.324 -12.055  42.907  1.00 25.99      D
ATOM   8688  C   HIS D 670     122.918 -15.176  47.326  1.00 27.14      D
ATOM   8689  O   HIS D 670     123.583 -15.346  48.362  1.00 25.08      D
ATOM   8690  N   THR D 671     122.059 -16.080  46.840  1.00 28.13      D
ATOM   8691  CA  THR D 671     121.796 -17.381  47.473  1.00 27.79      D
```

```
ATOM   8692  CB  THR D 671     121.180 -18.369  46.454  1.00 26.12      D
ATOM   8693  OG1 THR D 671     119.789 -18.069  46.289  1.00 23.95      D
ATOM   8694  CG2 THR D 671     121.312 -19.791  46.930  1.00 26.83      D
ATOM   8695  C   THR D 671     122.992 -18.034  48.162  1.00 29.31      D
ATOM   8696  O   THR D 671     122.854 -18.547  49.271  1.00 29.25      D
ATOM   8697  N   ASN D 672     124.156 -18.025  47.516  1.00 31.23      D
ATOM   8698  CA  ASN D 672     125.354 -18.627  48.116  1.00 33.42      D
ATOM   8699  CB  ASN D 672     126.498 -18.738  47.089  1.00 35.89      D
ATOM   8700  CG  ASN D 672     126.323 -19.911  46.105  1.00 40.95      D
ATOM   8701  OD1 ASN D 672     125.241 -20.116  45.535  1.00 42.75      D
ATOM   8702  ND2 ASN D 672     127.406 -20.672  45.887  1.00 42.55      D
ATOM   8703  C   ASN D 672     125.861 -17.813  49.317  1.00 33.48      D
ATOM   8704  O   ASN D 672     126.666 -18.302  50.105  1.00 35.72      D
ATOM   8705  N   LEU D 673     125.405 -16.574  49.455  1.00 31.40      D
ATOM   8706  CA  LEU D 673     125.864 -15.722  50.549  1.00 30.75      D
ATOM   8707  CB  LEU D 673     125.631 -16.410  51.901  1.00 30.83      D
ATOM   8708  CG  LEU D 673     124.165 -16.514  52.344  1.00 31.99      D
ATOM   8709  CD1 LEU D 673     124.059 -17.284  53.649  1.00 32.25      D
ATOM   8710  CD2 LEU D 673     123.580 -15.115  52.510  1.00 33.43      D
ATOM   8711  C   LEU D 673     127.346 -15.337  50.420  1.00 28.49      D
ATOM   8712  O   LEU D 673     128.045 -15.214  51.429  1.00 29.31      D
ATOM   8713  N   SER D 674     127.812 -15.145  49.185  1.00 24.89      D
ATOM   8714  CA  SER D 674     129.201 -14.771  48.911  1.00 23.72      D
ATOM   8715  CB  SER D 674     129.764 -15.608  47.764  1.00 23.54      D
ATOM   8716  OG  SER D 674     128.969 -15.454  46.598  1.00 27.66      D
ATOM   8717  C   SER D 674     129.289 -13.287  48.546  1.00 22.55      D
ATOM   8718  O   SER D 674     128.336 -12.721  48.035  1.00 22.93      D
ATOM   8719  N   ALA D 675     130.431 -12.657  48.796  1.00 21.17      D
ATOM   8720  CA  ALA D 675     130.580 -11.240  48.498  1.00 20.35      D
ATOM   8721  CB  ALA D 675     132.002 -10.779  48.814  1.00 16.29      D
ATOM   8722  C   ALA D 675     130.215 -10.836  47.075  1.00 20.97      D
ATOM   8723  O   ALA D 675     130.528 -11.527  46.095  1.00 22.46      D
ATOM   8724  N   ILE D 676     129.538  -9.703  46.972  1.00 21.38      D
ATOM   8725  CA  ILE D 676     129.180  -9.194  45.667  1.00 23.44      D
ATOM   8726  CB  ILE D 676     128.051  -8.132  45.734  1.00 24.56      D
ATOM   8727  CG2 ILE D 676     127.897  -7.484  44.377  1.00 23.13      D
ATOM   8728  CG1 ILE D 676     126.727  -8.776  46.197  1.00 25.69      D
ATOM   8729  CD1 ILE D 676     126.316 -10.018  45.386  1.00 25.28      D
ATOM   8730  C   ILE D 676     130.470  -8.526  45.202  1.00 23.09      D
ATOM   8731  O   ILE D 676     130.971  -7.613  45.853  1.00 23.97      D
ATOM   8732  N   THR D 677     131.012  -9.000  44.091  1.00 21.72      D
ATOM   8733  CA  THR D 677     132.250  -8.474  43.554  1.00 21.86      D
ATOM   8734  CB  THR D 677     133.096  -9.589  42.896  1.00 25.37      D
ATOM   8735  OG1 THR D 677     133.515 -10.542  43.884  1.00 25.75      D
ATOM   8736  CG2 THR D 677     134.328  -8.977  42.219  1.00 27.86      D
ATOM   8737  C   THR D 677     132.001  -7.420  42.488  1.00 20.83      D
ATOM   8738  O   THR D 677     132.880  -6.605  42.208  1.00 17.53      D
ATOM   8739  N   THR D 678     130.818  -7.457  41.876  1.00 20.52      D
ATOM   8740  CA  THR D 678     130.492  -6.512  40.821  1.00 19.25      D
ATOM   8741  CB  THR D 678     131.294  -6.864  39.512  1.00 20.24      D
ATOM   8742  OG1 THR D 678     131.093  -5.842  38.533  1.00 19.49      D
ATOM   8743  CG2 THR D 678     130.834  -8.193  38.927  1.00 17.27      D
ATOM   8744  C   THR D 678     129.001  -6.490  40.495  1.00 18.40      D
ATOM   8745  O   THR D 678     128.308  -7.497  40.627  1.00 17.73      D
```

```
ATOM   8746  N   PHE D 679     128.521  -5.336  40.044  1.00 19.50      D
ATOM   8747  CA  PHE D 679     127.119  -5.179  39.653  1.00 20.10      D
ATOM   8748  CB  PHE D 679     126.212  -5.151  40.896  1.00 19.62      D
ATOM   8749  CG  PHE D 679     126.072  -3.794  41.546  1.00 20.58      D
ATOM   8750  CD1 PHE D 679     125.187  -2.838  41.036  1.00 19.81      D
ATOM   8751  CD2 PHE D 679     126.786  -3.493  42.708  1.00 22.11      D
ATOM   8752  CE1 PHE D 679     125.008  -1.595  41.679  1.00 19.56      D
ATOM   8753  CE2 PHE D 679     126.622  -2.255  43.369  1.00 21.42      D
ATOM   8754  CZ  PHE D 679     125.730  -1.305  42.855  1.00 20.49      D
ATOM   8755  C   PHE D 679     126.967  -3.908  38.836  1.00 18.56      D
ATOM   8756  O   PHE D 679     127.824  -3.040  38.902  1.00 18.64      D
ATOM   8757  N   TYR D 680     125.900  -3.826  38.038  1.00 18.73      D
ATOM   8758  CA  TYR D 680     125.610  -2.640  37.216  1.00 18.62      D
ATOM   8759  CB  TYR D 680     126.140  -2.818  35.776  1.00 19.64      D
ATOM   8760  CG  TYR D 680     126.416  -1.498  35.070  1.00 21.94      D
ATOM   8761  CD1 TYR D 680     127.503  -0.704  35.447  1.00 21.42      D
ATOM   8762  CE1 TYR D 680     127.691   0.578  34.917  1.00 21.58      D
ATOM   8763  CD2 TYR D 680     125.525  -0.982  34.123  1.00 21.80      D
ATOM   8764  CE2 TYR D 680     125.702   0.304  33.585  1.00 21.45      D
ATOM   8765  CZ  TYR D 680     126.780   1.083  33.992  1.00 21.61      D
ATOM   8766  OH  TYR D 680     126.891   2.384  33.541  1.00 21.38      D
ATOM   8767  C   TYR D 680     124.087  -2.429  37.194  1.00 18.89      D
ATOM   8768  O   TYR D 680     123.326  -3.394  37.244  1.00 21.29      D
ATOM   8769  N   VAL D 681     123.635  -1.182  37.148  1.00 18.55      D
ATOM   8770  CA  VAL D 681     122.202  -0.952  37.112  1.00 20.06      D
ATOM   8771  CB  VAL D 681     121.588  -0.612  38.502  1.00 19.46      D
ATOM   8772  CG1 VAL D 681     121.748  -1.770  39.427  1.00 23.82      D
ATOM   8773  CG2 VAL D 681     122.219   0.634  39.080  1.00 18.66      D
ATOM   8774  C   VAL D 681     121.699   0.134  36.196  1.00 21.12      D
ATOM   8775  O   VAL D 681     122.429   1.030  35.748  1.00 19.50      D
ATOM   8776  N   SER D 682     120.404   0.039  35.956  1.00 22.21      D
ATOM   8777  CA  SER D 682     119.698   0.991  35.147  1.00 21.87      D
ATOM   8778  CB  SER D 682     119.633   0.520  33.703  1.00 20.44      D
ATOM   8779  OG  SER D 682     118.589  -0.410  33.525  1.00 21.95      D
ATOM   8780  C   SER D 682     118.331   0.950  35.783  1.00 23.11      D
ATOM   8781  O   SER D 682     118.048   0.053  36.582  1.00 22.65      D
ATOM   8782  N   ASP D 683     117.483   1.910  35.457  1.00 23.07      D
ATOM   8783  CA  ASP D 683     116.165   1.901  36.050  1.00 23.72      D
ATOM   8784  CB  ASP D 683     115.359   3.107  35.591  1.00 26.85      D
ATOM   8785  CG  ASP D 683     115.822   4.384  36.224  1.00 30.20      D
ATOM   8786  OD1 ASP D 683     116.151   4.341  37.431  1.00 35.54      D
ATOM   8787  OD2 ASP D 683     115.840   5.421  35.521  1.00 28.97      D
ATOM   8788  C   ASP D 683     115.381   0.631  35.728  1.00 22.90      D
ATOM   8789  O   ASP D 683     114.466   0.281  36.458  1.00 22.58      D
ATOM   8790  N   ASN D 684     115.717  -0.072  34.653  1.00 21.68      D
ATOM   8791  CA  ASN D 684     114.937  -1.257  34.335  1.00 21.96      D
ATOM   8792  CB  ASN D 684     114.568  -1.291  32.842  1.00 20.91      D
ATOM   8793  CG  ASN D 684     113.639  -0.138  32.417  1.00 22.88      D
ATOM   8794  OD1 ASN D 684     112.685   0.229  33.132  1.00 20.08      D
ATOM   8795  ND2 ASN D 684     113.907   0.423  31.231  1.00 21.27      D
ATOM   8796  C   ASN D 684     115.561  -2.597  34.705  1.00 22.28      D
ATOM   8797  O   ASN D 684     114.840  -3.557  34.983  1.00 21.62      D
ATOM   8798  N   ILE D 685     116.890  -2.659  34.735  1.00 22.22      D
ATOM   8799  CA  ILE D 685     117.592  -3.906  35.022  1.00 24.26      D
```

```
ATOM   8800  CB  ILE D 685     118.241  -4.431  33.725  1.00 25.72      D
ATOM   8801  CG2 ILE D 685     119.014  -5.722  33.987  1.00 28.28      D
ATOM   8802  CG1 ILE D 685     117.181  -4.607  32.646  1.00 26.62      D
ATOM   8803  CD1 ILE D 685     117.527  -3.851  31.344  1.00 32.32      D
ATOM   8804  C   ILE D 685     118.701  -3.830  36.081  1.00 25.44      D
ATOM   8805  O   ILE D 685     119.291  -2.771  36.300  1.00 25.75      D
ATOM   8806  N   LEU D 686     118.989  -4.964  36.717  1.00 25.66      D
ATOM   8807  CA  LEU D 686     120.069  -5.041  37.689  1.00 26.90      D
ATOM   8808  CB  LEU D 686     119.530  -5.089  39.127  1.00 26.08      D
ATOM   8809  CG  LEU D 686     120.472  -5.572  40.262  1.00 23.99      D
ATOM   8810  CD1 LEU D 686     121.709  -4.699  40.345  1.00 23.40      D
ATOM   8811  CD2 LEU D 686     119.740  -5.567  41.585  1.00 21.28      D
ATOM   8812  C   LEU D 686     120.859  -6.317  37.412  1.00 28.01      D
ATOM   8813  O   LEU D 686     120.275  -7.397  37.340  1.00 28.42      D
ATOM   8814  N   VAL D 687     122.170  -6.194  37.226  1.00 26.81      D
ATOM   8815  CA  VAL D 687     122.995  -7.371  37.019  1.00 28.16      D
ATOM   8816  CB  VAL D 687     123.648  -7.401  35.629  1.00 28.88      D
ATOM   8817  CG1 VAL D 687     124.496  -8.669  35.484  1.00 27.76      D
ATOM   8818  CG2 VAL D 687     122.562  -7.383  34.553  1.00 29.55      D
ATOM   8819  C   VAL D 687     124.064  -7.347  38.098  1.00 29.32      D
ATOM   8820  O   VAL D 687     124.744  -6.331  38.291  1.00 29.09      D
ATOM   8821  N   SER D 688     124.200  -8.465  38.813  1.00 28.34      D
ATOM   8822  CA  SER D 688     125.166  -8.570  39.910  1.00 27.42      D
ATOM   8823  CB  SER D 688     124.419  -8.567  41.247  1.00 26.52      D
ATOM   8824  OG  SER D 688     123.505  -9.651  41.304  1.00 25.52      D
ATOM   8825  C   SER D 688     125.990  -9.853  39.808  1.00 27.67      D
ATOM   8826  O   SER D 688     125.518 -10.870  39.304  1.00 28.15      D
ATOM   8827  N   GLY D 689     127.217  -9.818  40.299  1.00 25.88      D
ATOM   8828  CA  GLY D 689     128.012 -11.016  40.228  1.00 25.97      D
ATOM   8829  C   GLY D 689     128.901 -11.218  41.422  1.00 27.10      D
ATOM   8830  O   GLY D 689     129.549 -10.285  41.890  1.00 29.72      D
ATOM   8831  N   SER D 690     128.914 -12.445  41.922  1.00 27.15      D
ATOM   8832  CA  SER D 690     129.752 -12.819  43.042  1.00 27.45      D
ATOM   8833  CB  SER D 690     128.918 -13.015  44.300  1.00 26.48      D
ATOM   8834  OG  SER D 690     127.975 -14.044  44.099  1.00 25.71      D
ATOM   8835  C   SER D 690     130.376 -14.145  42.630  1.00 28.76      D
ATOM   8836  O   SER D 690     130.435 -14.457  41.444  1.00 28.74      D
ATOM   8837  N   GLU D 691     130.829 -14.925  43.609  1.00 29.69      D
ATOM   8838  CA  GLU D 691     131.446 -16.210  43.320  1.00 29.80      D
ATOM   8839  CB  GLU D 691     132.241 -16.711  44.532  1.00 30.89      D
ATOM   8840  CG  GLU D 691     132.740 -18.153  44.426  1.00 34.76      D
ATOM   8841  CD  GLU D 691     133.806 -18.516  45.469  1.00 37.18      D
ATOM   8842  OE1 GLU D 691     134.895 -17.901  45.448  1.00 39.22      D
ATOM   8843  OE2 GLU D 691     133.564 -19.420  46.305  1.00 38.14      D
ATOM   8844  C   GLU D 691     130.409 -17.239  42.888  1.00 29.94      D
ATOM   8845  O   GLU D 691     129.441 -17.507  43.596  1.00 28.81      D
ATOM   8846  N   ASN D 692     130.621 -17.784  41.693  1.00 30.68      D
ATOM   8847  CA  ASN D 692     129.756 -18.800  41.122  1.00 30.63      D
ATOM   8848  CB  ASN D 692     129.854 -20.070  41.975  1.00 32.82      D
ATOM   8849  CG  ASN D 692     131.019 -20.951  41.562  1.00 34.81      D
ATOM   8850  OD1 ASN D 692     130.832 -21.908  40.812  1.00 39.00      D
ATOM   8851  ND2 ASN D 692     132.231 -20.614  42.016  1.00 34.40      D
ATOM   8852  C   ASN D 692     128.313 -18.370  40.941  1.00 30.73      D
ATOM   8853  O   ASN D 692     127.395 -19.187  40.996  1.00 31.82      D
```

```
ATOM   8854  N   GLN D 693     128.113 -17.081  40.711  1.00 30.83      D
ATOM   8855  CA  GLN D 693     126.774 -16.564  40.496  1.00 30.85      D
ATOM   8856  CB  GLN D 693     126.127 -16.215  41.837  1.00 32.95      D
ATOM   8857  CG  GLN D 693     125.494 -17.398  42.562  1.00 36.48      D
ATOM   8858  CD  GLN D 693     124.636 -16.949  43.741  1.00 39.48      D
ATOM   8859  OE1 GLN D 693     123.650 -16.222  43.571  1.00 40.51      D
ATOM   8860  NE2 GLN D 693     125.014 -17.371  44.941  1.00 40.67      D
ATOM   8861  C   GLN D 693     126.771 -15.350  39.560  1.00 30.20      D
ATOM   8862  O   GLN D 693     127.694 -14.533  39.586  1.00 28.95      D
ATOM   8863  N   PHE D 694     125.729 -15.268  38.728  1.00 28.92      D
ATOM   8864  CA  PHE D 694     125.534 -14.189  37.758  1.00 27.46      D
ATOM   8865  CB  PHE D 694     126.183 -14.549  36.404  1.00 26.85      D
ATOM   8866  CG  PHE D 694     126.212 -13.402  35.413  1.00 27.99      D
ATOM   8867  CD1 PHE D 694     127.027 -12.290  35.626  1.00 28.31      D
ATOM   8868  CD2 PHE D 694     125.387 -13.411  34.291  1.00 28.25      D
ATOM   8869  CE1 PHE D 694     127.011 -11.201  34.734  1.00 25.87      D
ATOM   8870  CE2 PHE D 694     125.365 -12.329  33.397  1.00 26.35      D
ATOM   8871  CZ  PHE D 694     126.175 -11.226  33.620  1.00 24.43      D
ATOM   8872  C   PHE D 694     124.018 -14.020  37.600  1.00 26.65      D
ATOM   8873  O   PHE D 694     123.360 -14.804  36.923  1.00 27.90      D
ATOM   8874  N   ASN D 695     123.462 -12.997  38.235  1.00 25.11      D
ATOM   8875  CA  ASN D 695     122.033 -12.784  38.169  1.00 22.66      D
ATOM   8876  CB  ASN D 695     121.462 -12.735  39.570  1.00 21.74      D
ATOM   8877  CG  ASN D 695     121.802 -13.948  40.351  1.00 22.53      D
ATOM   8878  OD1 ASN D 695     122.469 -13.863  41.381  1.00 25.44      D
ATOM   8879  ND2 ASN D 695     121.369 -15.102  39.866  1.00 21.60      D
ATOM   8880  C   ASN D 695     121.586 -11.557  37.431  1.00 22.56      D
ATOM   8881  O   ASN D 695     122.283 -10.537  37.402  1.00 24.25      D
ATOM   8882  N   ILE D 696     120.407 -11.675  36.828  1.00 20.27      D
ATOM   8883  CA  ILE D 696     119.785 -10.570  36.112  1.00 18.17      D
ATOM   8884  CB  ILE D 696     119.741 -10.848  34.598  1.00 13.96      D
ATOM   8885  CG2 ILE D 696     119.173  -9.631  33.874  1.00 12.40      D
ATOM   8886  CG1 ILE D 696     121.165 -11.096  34.095  1.00 11.96      D
ATOM   8887  CD1 ILE D 696     121.278 -11.411  32.627  1.00 10.15      D
ATOM   8888  C   ILE D 696     118.375 -10.387  36.708  1.00 19.43      D
ATOM   8889  O   ILE D 696     117.558 -11.307  36.714  1.00 19.49      D
ATOM   8890  N   TYR D 697     118.130  -9.194  37.236  1.00 18.77      D
ATOM   8891  CA  TYR D 697     116.878  -8.867  37.881  1.00 17.94      D
ATOM   8892  CB  TYR D 697     117.167  -8.295  39.280  1.00 19.60      D
ATOM   8893  CG  TYR D 697     118.014  -9.185  40.171  1.00 19.57      D
ATOM   8894  CD1 TYR D 697     117.428 -10.186  40.962  1.00 20.99      D
ATOM   8895  CE1 TYR D 697     118.204 -11.012  41.789  1.00 18.57      D
ATOM   8896  CD2 TYR D 697     119.397  -9.031  40.223  1.00 18.67      D
ATOM   8897  CE2 TYR D 697     120.179  -9.840  41.035  1.00 19.21      D
ATOM   8898  CZ  TYR D 697     119.581 -10.832  41.820  1.00 20.43      D
ATOM   8899  OH  TYR D 697     120.372 -11.634  42.627  1.00 20.44      D
ATOM   8900  C   TYR D 697     116.059  -7.843  37.104  1.00 18.57      D
ATOM   8901  O   TYR D 697     116.604  -6.934  36.456  1.00 18.53      D
ATOM   8902  N   ASN D 698     114.746  -7.975  37.208  1.00 16.25      D
ATOM   8903  CA  ASN D 698     113.826  -7.049  36.575  1.00 16.13      D
ATOM   8904  CB  ASN D 698     112.594  -7.832  36.111  1.00 16.70      D
ATOM   8905  CG  ASN D 698     111.516  -6.939  35.508  1.00 18.93      D
ATOM   8906  OD1 ASN D 698     111.253  -5.822  36.004  1.00 16.72      D
ATOM   8907  ND2 ASN D 698     110.873  -7.428  34.443  1.00 16.48      D
```

```
ATOM   8908  C   ASN D 698     113.441  -6.032  37.682  1.00 15.83      D
ATOM   8909  O   ASN D 698     112.568  -6.301  38.499  1.00 14.84      D
ATOM   8910  N   LEU D 699     114.078  -4.874  37.735  1.00 14.22      D
ATOM   8911  CA  LEU D 699     113.725  -3.948  38.796  1.00 15.47      D
ATOM   8912  CB  LEU D 699     114.549  -2.673  38.704  1.00 11.67      D
ATOM   8913  CG  LEU D 699     115.818  -2.596  39.541  1.00 12.58      D
ATOM   8914  CD1 LEU D 699     116.357  -4.000  39.957  1.00  9.17      D
ATOM   8915  CD2 LEU D 699     116.822  -1.809  38.724  1.00  9.81      D
ATOM   8916  C   LEU D 699     112.260  -3.560  38.883  1.00 18.10      D
ATOM   8917  O   LEU D 699     111.836  -3.053  39.914  1.00 21.11      D
ATOM   8918  N   ARG D 700     111.479  -3.765  37.826  1.00 19.06      D
ATOM   8919  CA  ARG D 700     110.063  -3.382  37.889  1.00 18.41      D
ATOM   8920  CB  ARG D 700     109.474  -3.190  36.481  1.00 16.13      D
ATOM   8921  CG  ARG D 700     110.078  -2.053  35.660  1.00 18.32      D
ATOM   8922  CD  ARG D 700     109.605  -2.100  34.188  1.00 19.47      D
ATOM   8923  NE  ARG D 700     110.340  -1.195  33.295  1.00 19.60      D
ATOM   8924  CZ  ARG D 700     109.881  -0.738  32.127  1.00 20.84      D
ATOM   8925  NH1 ARG D 700     108.678  -1.085  31.693  1.00 19.16      D
ATOM   8926  NH2 ARG D 700     110.633   0.057  31.378  1.00 20.52      D
ATOM   8927  C   ARG D 700     109.211  -4.411  38.652  1.00 19.19      D
ATOM   8928  O   ARG D 700     108.440  -4.069  39.546  1.00 20.01      D
ATOM   8929  N   SER D 701     109.344  -5.673  38.286  1.00 18.61      D
ATOM   8930  CA  SER D 701     108.580  -6.719  38.919  1.00 18.99      D
ATOM   8931  CB  SER D 701     108.403  -7.907  37.960  1.00 17.26      D
ATOM   8932  OG  SER D 701     109.627  -8.299  37.350  1.00 16.41      D
ATOM   8933  C   SER D 701     109.317  -7.179  40.154  1.00 21.34      D
ATOM   8934  O   SER D 701     108.758  -7.881  40.983  1.00 21.67      D
ATOM   8935  N   GLY D 702     110.577  -6.782  40.277  1.00 23.17      D
ATOM   8936  CA  GLY D 702     111.367  -7.189  41.420  1.00 25.46      D
ATOM   8937  C   GLY D 702     111.916  -8.601  41.338  1.00 26.82      D
ATOM   8938  O   GLY D 702     112.676  -9.008  42.208  1.00 28.70      D
ATOM   8939  N   LYS D 703     111.580  -9.346  40.290  1.00 28.39      D
ATOM   8940  CA  LYS D 703     112.040 -10.734  40.187  1.00 29.97      D
ATOM   8941  CB  LYS D 703     110.926 -11.616  39.609  1.00 30.86      D
ATOM   8942  CG  LYS D 703     109.566 -11.294  40.211  1.00 34.24      D
ATOM   8943  CD  LYS D 703     108.553 -12.393  40.031  1.00 36.04      D
ATOM   8944  CE  LYS D 703     108.971 -13.657  40.786  1.00 38.38      D
ATOM   8945  NZ  LYS D 703     107.900 -14.711  40.780  1.00 39.62      D
ATOM   8946  C   LYS D 703     113.319 -11.022  39.428  1.00 30.16      D
ATOM   8947  O   LYS D 703     113.822 -10.202  38.665  1.00 33.16      D
ATOM   8948  N   LEU D 704     113.824 -12.227  39.655  1.00 31.22      D
ATOM   8949  CA  LEU D 704     115.037 -12.717  39.024  1.00 31.13      D
ATOM   8950  CB  LEU D 704     115.655 -13.799  39.894  1.00 28.59      D
ATOM   8951  CG  LEU D 704     116.959 -14.425  39.433  1.00 29.39      D
ATOM   8952  CD1 LEU D 704     118.092 -13.385  39.446  1.00 31.25      D
ATOM   8953  CD2 LEU D 704     117.298 -15.548  40.368  1.00 27.62      D
ATOM   8954  C   LEU D 704     114.663 -13.302  37.668  1.00 32.42      D
ATOM   8955  O   LEU D 704     113.791 -14.167  37.585  1.00 34.11      D
ATOM   8956  N   VAL D 705     115.308 -12.827  36.607  1.00 32.96      D
ATOM   8957  CA  VAL D 705     115.014 -13.329  35.275  1.00 33.27      D
ATOM   8958  CB  VAL D 705     115.052 -12.240  34.214  1.00 31.84      D
ATOM   8959  CG1 VAL D 705     114.710 -12.853  32.866  1.00 33.49      D
ATOM   8960  CG2 VAL D 705     114.079 -11.142  34.544  1.00 30.65      D
ATOM   8961  C   VAL D 705     116.011 -14.389  34.841  1.00 35.05      D
```

```
ATOM   8962  O   VAL D 705     115.632 -15.501  34.504  1.00 37.11      D
ATOM   8963  N   HIS D 706     117.291 -14.041  34.827  1.00 36.45      D
ATOM   8964  CA  HIS D 706     118.316 -14.991  34.426  1.00 36.74      D
ATOM   8965  CB  HIS D 706     119.007 -14.539  33.137  1.00 37.71      D
ATOM   8966  CG  HIS D 706     118.064 -14.142  32.042  1.00 40.20      D
ATOM   8967  CD2 HIS D 706     117.901 -12.964  31.392  1.00 41.01      D
ATOM   8968  ND1 HIS D 706     117.172 -15.022  31.468  1.00 40.45      D
ATOM   8969  CE1 HIS D 706     116.504 -14.404  30.509  1.00 41.40      D
ATOM   8970  NE2 HIS D 706     116.927 -13.155  30.441  1.00 41.00      D
ATOM   8971  C   HIS D 706     119.361 -15.155  35.527  1.00 37.89      D
ATOM   8972  O   HIS D 706     119.869 -14.174  36.096  1.00 38.65      D
ATOM   8973  N   ALA D 707     119.686 -16.414  35.805  1.00 37.80      D
ATOM   8974  CA  ALA D 707     120.660 -16.757  36.828  1.00 36.66      D
ATOM   8975  CB  ALA D 707     119.935 -17.223  38.075  1.00 33.53      D
ATOM   8976  C   ALA D 707     121.651 -17.828  36.367  1.00 36.44      D
ATOM   8977  O   ALA D 707     122.608 -18.138  37.079  1.00 36.66      D
ATOM   8978  N   ASN D 708     121.446 -18.382  35.177  1.00 36.37      D
ATOM   8979  CA  ASN D 708     122.347 -19.431  34.710  1.00 37.18      D
ATOM   8980  CB  ASN D 708     121.553 -20.739  34.521  1.00 37.73      D
ATOM   8981  CG  ASN D 708     120.893 -21.212  35.821  1.00 38.57      D
ATOM   8982  OD1 ASN D 708     119.667 -21.227  35.947  1.00 38.35      D
ATOM   8983  ND2 ASN D 708     121.712 -21.588  36.794  1.00 37.37      D
ATOM   8984  C   ASN D 708     123.137 -19.084  33.443  1.00 36.59      D
ATOM   8985  O   ASN D 708     123.856 -19.927  32.907  1.00 35.29      D
ATOM   8986  N   ILE D 709     123.019 -17.839  32.986  1.00 35.82      D
ATOM   8987  CA  ILE D 709     123.709 -17.402  31.781  1.00 34.43      D
ATOM   8988  CB  ILE D 709     123.349 -15.928  31.408  1.00 32.34      D
ATOM   8989  CG2 ILE D 709     124.151 -15.460  30.221  1.00 30.43      D
ATOM   8990  CG1 ILE D 709     121.875 -15.836  31.017  1.00 30.65      D
ATOM   8991  CD1 ILE D 709     121.444 -14.459  30.565  1.00 28.79      D
ATOM   8992  C   ILE D 709     125.216 -17.552  31.873  1.00 34.88      D
ATOM   8993  O   ILE D 709     125.863 -17.878  30.882  1.00 36.86      D
ATOM   8994  N   LEU D 710     125.785 -17.336  33.051  1.00 34.63      D
ATOM   8995  CA  LEU D 710     127.232 -17.454  33.186  1.00 32.46      D
ATOM   8996  CB  LEU D 710     127.837 -16.058  33.402  1.00 28.39      D
ATOM   8997  CG  LEU D 710     128.450 -15.306  32.208  1.00 25.87      D
ATOM   8998  CD1 LEU D 710     127.798 -15.707  30.894  1.00 24.33      D
ATOM   8999  CD2 LEU D 710     128.331 -13.810  32.443  1.00 23.04      D
ATOM   9000  C   LEU D 710     127.683 -18.434  34.269  1.00 33.52      D
ATOM   9001  O   LEU D 710     128.730 -18.246  34.882  1.00 34.43      D
ATOM   9002  N   LYS D 711     126.902 -19.494  34.480  1.00 34.36      D
ATOM   9003  CA  LYS D 711     127.230 -20.518  35.481  1.00 35.44      D
ATOM   9004  CB  LYS D 711     126.238 -21.670  35.389  1.00 34.96      D
ATOM   9005  CG  LYS D 711     125.872 -22.006  33.980  1.00 36.79      D
ATOM   9006  CD  LYS D 711     124.620 -22.834  33.940  1.00 38.39      D
ATOM   9007  CE  LYS D 711     124.936 -24.285  34.192  1.00 40.21      D
ATOM   9008  NZ  LYS D 711     125.841 -24.794  33.104  1.00 42.27      D
ATOM   9009  C   LYS D 711     128.645 -21.068  35.350  1.00 36.53      D
ATOM   9010  O   LYS D 711     129.284 -21.427  36.341  1.00 36.63      D
ATOM   9011  N   ASP D 712     129.130 -21.126  34.121  1.00 37.64      D
ATOM   9012  CA  ASP D 712     130.457 -21.629  33.836  1.00 39.74      D
ATOM   9013  CB  ASP D 712     130.688 -21.555  32.336  1.00 44.17      D
ATOM   9014  CG  ASP D 712     129.490 -22.032  31.558  1.00 49.91      D
ATOM   9015  OD1 ASP D 712     129.338 -23.276  31.408  1.00 53.21      D
```

```
ATOM   9016  OD2 ASP D 712     128.684 -21.163  31.122  1.00 51.40      D
ATOM   9017  C   ASP D 712     131.548 -20.856  34.551  1.00 39.02      D
ATOM   9018  O   ASP D 712     132.528 -21.439  34.992  1.00 39.79      D
ATOM   9019  N   ALA D 713     131.398 -19.542  34.647  1.00 37.44      D
ATOM   9020  CA  ALA D 713     132.427 -18.740  35.295  1.00 37.31      D
ATOM   9021  CB  ALA D 713     132.131 -17.254  35.119  1.00 37.40      D
ATOM   9022  C   ALA D 713     132.603 -19.055  36.775  1.00 36.89      D
ATOM   9023  O   ALA D 713     131.693 -19.535  37.437  1.00 37.66      D
ATOM   9024  N   ASP D 714     133.785 -18.782  37.296  1.00 35.36      D
ATOM   9025  CA  ASP D 714     134.018 -19.033  38.693  1.00 34.87      D
ATOM   9026  CB  ASP D 714     135.384 -19.678  38.893  1.00 33.94      D
ATOM   9027  CG  ASP D 714     135.484 -21.038  38.244  1.00 32.23      D
ATOM   9028  OD1 ASP D 714     134.599 -21.877  38.477  1.00 32.51      D
ATOM   9029  OD2 ASP D 714     136.456 -21.279  37.505  1.00 34.54      D
ATOM   9030  C   ASP D 714     133.946 -17.705  39.433  1.00 35.72      D
ATOM   9031  O   ASP D 714     133.610 -17.651  40.616  1.00 35.20      D
ATOM   9032  N   GLN D 715     134.238 -16.629  38.714  1.00 35.93      D
ATOM   9033  CA  GLN D 715     134.233 -15.293  39.284  1.00 36.18      D
ATOM   9034  CB  GLN D 715     135.648 -14.938  39.750  1.00 37.10      D
ATOM   9035  CG  GLN D 715     136.260 -15.951  40.716  1.00 39.05      D
ATOM   9036  CD  GLN D 715     135.897 -15.672  42.165  1.00 40.12      D
ATOM   9037  OE1 GLN D 715     134.751 -15.380  42.472  1.00 42.68      D
ATOM   9038  NE2 GLN D 715     136.874 -15.763  43.057  1.00 39.97      D
ATOM   9039  C   GLN D 715     133.756 -14.264  38.254  1.00 35.81      D
ATOM   9040  O   GLN D 715     133.993 -14.407  37.054  1.00 35.76      D
ATOM   9041  N   ILE D 716     133.073 -13.232  38.736  1.00 34.56      D
ATOM   9042  CA  ILE D 716     132.582 -12.149  37.888  1.00 32.51      D
ATOM   9043  CB  ILE D 716     131.061 -11.982  38.032  1.00 31.79      D
ATOM   9044  CG2 ILE D 716     130.547 -11.006  36.996  1.00 30.49      D
ATOM   9045  CG1 ILE D 716     130.363 -13.336  37.890  1.00 33.24      D
ATOM   9046  CD1 ILE D 716     130.638 -14.060  36.579  1.00 34.30      D
ATOM   9047  C   ILE D 716     133.285 -10.863  38.375  1.00 32.59      D
ATOM   9048  O   ILE D 716     132.797 -10.160  39.264  1.00 33.77      D
ATOM   9049  N   TRP D 717     134.444 -10.580  37.795  1.00 30.84      D
ATOM   9050  CA  TRP D 717     135.252  -9.429  38.162  1.00 29.11      D
ATOM   9051  CB  TRP D 717     136.558  -9.454  37.379  1.00 32.71      D
ATOM   9052  CG  TRP D 717     137.348 -10.687  37.596  1.00 35.43      D
ATOM   9053  CD2 TRP D 717     137.669 -11.278  38.855  1.00 35.53      D
ATOM   9054  CE2 TRP D 717     138.462 -12.416  38.589  1.00 36.83      D
ATOM   9055  CE3 TRP D 717     137.364 -10.960  40.185  1.00 35.83      D
ATOM   9056  CD1 TRP D 717     137.940 -11.464  36.640  1.00 36.35      D
ATOM   9057  NE1 TRP D 717     138.612 -12.504  37.230  1.00 37.07      D
ATOM   9058  CZ2 TRP D 717     138.956 -13.237  39.605  1.00 38.32      D
ATOM   9059  CZ3 TRP D 717     137.855 -11.780  41.193  1.00 37.12      D
ATOM   9060  CH2 TRP D 717     138.641 -12.904  40.896  1.00 37.38      D
ATOM   9061  C   TRP D 717     134.583  -8.102  37.930  1.00 26.79      D
ATOM   9062  O   TRP D 717     134.507  -7.262  38.825  1.00 24.62      D
ATOM   9063  N   SER D 718     134.110  -7.899  36.713  1.00 24.96      D
ATOM   9064  CA  SER D 718     133.473  -6.639  36.403  1.00 23.33      D
ATOM   9065  CB  SER D 718     134.499  -5.674  35.830  1.00 21.39      D
ATOM   9066  OG  SER D 718     133.898  -4.420  35.620  1.00 24.14      D
ATOM   9067  C   SER D 718     132.347  -6.825  35.421  1.00 22.63      D
ATOM   9068  O   SER D 718     132.481  -7.549  34.443  1.00 25.60      D
ATOM   9069  N   VAL D 719     131.228  -6.175  35.679  1.00 21.31      D
```

```
ATOM   9070  CA  VAL D 719     130.095  -6.286  34.784  1.00 23.17      D
ATOM   9071  CB  VAL D 719     128.900  -6.926  35.517  1.00 23.18      D
ATOM   9072  CG1 VAL D 719     128.244  -5.916  36.483  1.00 23.48      D
ATOM   9073  CG2 VAL D 719     127.915  -7.427  34.517  1.00 24.77      D
ATOM   9074  C   VAL D 719     129.703  -4.887  34.255  1.00 24.78      D
ATOM   9075  O   VAL D 719     130.024  -3.864  34.872  1.00 25.63      D
ATOM   9076  N   ASN D 720     129.005  -4.835  33.125  1.00 25.17      D
ATOM   9077  CA  ASN D 720     128.604  -3.547  32.543  1.00 25.66      D
ATOM   9078  CB  ASN D 720     129.844  -2.787  31.999  1.00 25.58      D
ATOM   9079  CG  ASN D 720     129.627  -1.256  31.853  1.00 26.08      D
ATOM   9080  OD1 ASN D 720     128.697  -0.790  31.193  1.00 24.37      D
ATOM   9081  ND2 ASN D 720     130.527  -0.484  32.456  1.00 24.14      D
ATOM   9082  C   ASN D 720     127.665  -3.882  31.397  1.00 25.69      D
ATOM   9083  O   ASN D 720     127.961  -4.770  30.601  1.00 24.75      D
ATOM   9084  N   PHE D 721     126.524  -3.209  31.324  1.00 25.70      D
ATOM   9085  CA  PHE D 721     125.610  -3.473  30.226  1.00 25.92      D
ATOM   9086  CB  PHE D 721     124.486  -4.426  30.663  1.00 24.85      D
ATOM   9087  CG  PHE D 721     123.483  -3.803  31.566  1.00 23.85      D
ATOM   9088  CD1 PHE D 721     122.441  -3.052  31.043  1.00 22.92      D
ATOM   9089  CD2 PHE D 721     123.588  -3.938  32.941  1.00 22.57      D
ATOM   9090  CE1 PHE D 721     121.525  -2.442  31.877  1.00 21.91      D
ATOM   9091  CE2 PHE D 721     122.675  -3.328  33.777  1.00 22.55      D
ATOM   9092  CZ  PHE D 721     121.640  -2.579  33.243  1.00 21.48      D
ATOM   9093  C   PHE D 721     125.076  -2.145  29.706  1.00 26.21      D
ATOM   9094  O   PHE D 721     125.149  -1.120  30.402  1.00 25.17      D
ATOM   9095  N   LYS D 722     124.564  -2.166  28.473  1.00 26.41      D
ATOM   9096  CA  LYS D 722     124.046  -0.966  27.801  1.00 25.77      D
ATOM   9097  CB  LYS D 722     125.230  -0.140  27.287  1.00 25.66      D
ATOM   9098  CG  LYS D 722     125.220   1.340  27.627  1.00 26.55      D
ATOM   9099  CD  LYS D 722     124.193   2.106  26.828  1.00 28.07      D
ATOM   9100  CE  LYS D 722     124.609   3.586  26.571  1.00 31.04      D
ATOM   9101  NZ  LYS D 722     125.623   3.789  25.462  1.00 31.59      D
ATOM   9102  C   LYS D 722     123.152  -1.376  26.621  1.00 25.54      D
ATOM   9103  O   LYS D 722     123.556  -2.161  25.765  1.00 24.73      D
ATOM   9104  N   GLY D 723     121.936  -0.851  26.580  1.00 25.69      D
ATOM   9105  CA  GLY D 723     121.044  -1.201  25.497  1.00 25.26      D
ATOM   9106  C   GLY D 723     120.804  -2.694  25.431  1.00 27.03      D
ATOM   9107  O   GLY D 723     120.226  -3.287  26.342  1.00 28.21      D
ATOM   9108  N   LYS D 724     121.262  -3.313  24.350  1.00 28.66      D
ATOM   9109  CA  LYS D 724     121.087  -4.752  24.144  1.00 29.79      D
ATOM   9110  CB  LYS D 724     120.590  -4.978  22.732  1.00 30.45      D
ATOM   9111  CG  LYS D 724     121.344  -4.146  21.713  1.00 32.48      D
ATOM   9112  CD  LYS D 724     122.379  -4.944  20.947  1.00 34.54      D
ATOM   9113  CE  LYS D 724     122.796  -4.163  19.693  1.00 36.42      D
ATOM   9114  NZ  LYS D 724     123.789  -4.878  18.817  1.00 36.97      D
ATOM   9115  C   LYS D 724     122.373  -5.535  24.346  1.00 29.03      D
ATOM   9116  O   LYS D 724     122.417  -6.749  24.142  1.00 28.40      D
ATOM   9117  N   THR D 725     123.409  -4.820  24.759  1.00 28.23      D
ATOM   9118  CA  THR D 725     124.720  -5.400  24.964  1.00 27.95      D
ATOM   9119  CB  THR D 725     125.784  -4.578  24.178  1.00 27.43      D
ATOM   9120  OG1 THR D 725     125.351  -4.417  22.821  1.00 26.72      D
ATOM   9121  CG2 THR D 725     127.134  -5.273  24.189  1.00 25.82      D
ATOM   9122  C   THR D 725     125.106  -5.460  26.443  1.00 27.90      D
ATOM   9123  O   THR D 725     124.891  -4.505  27.199  1.00 28.70      D
```

```
ATOM   9124  N   LEU D 726     125.682  -6.591  26.842  1.00 26.83      D
ATOM   9125  CA  LEU D 726     126.119  -6.806  28.213  1.00 24.94      D
ATOM   9126  CB  LEU D 726     125.126  -7.703  28.937  1.00 27.71      D
ATOM   9127  CG  LEU D 726     125.632  -8.393  30.211  1.00 29.98      D
ATOM   9128  CD1 LEU D 726     126.114  -7.390  31.271  1.00 30.93      D
ATOM   9129  CD2 LEU D 726     124.478  -9.202  30.758  1.00 31.05      D
ATOM   9130  C   LEU D 726     127.485  -7.441  28.245  1.00 22.94      D
ATOM   9131  O   LEU D 726     127.673  -8.537  27.741  1.00 24.07      D
ATOM   9132  N   VAL D 727     128.436  -6.753  28.856  1.00 23.62      D
ATOM   9133  CA  VAL D 727     129.798  -7.256  28.940  1.00 23.62      D
ATOM   9134  CB  VAL D 727     130.766  -6.218  28.377  1.00 24.57      D
ATOM   9135  CG1 VAL D 727     132.189  -6.737  28.490  1.00 28.26      D
ATOM   9136  CG2 VAL D 727     130.414  -5.939  26.896  1.00 22.22      D
ATOM   9137  C   VAL D 727     130.214  -7.625  30.360  1.00 21.59      D
ATOM   9138  O   VAL D 727     129.738  -7.034  31.333  1.00 20.77      D
ATOM   9139  N   ALA D 728     131.106  -8.608  30.461  1.00 21.47      D
ATOM   9140  CA  ALA D 728     131.597  -9.084  31.751  1.00 21.74      D
ATOM   9141  CB  ALA D 728     130.593 -10.057  32.371  1.00 23.07      D
ATOM   9142  C   ALA D 728     132.952  -9.749  31.692  1.00 21.99      D
ATOM   9143  O   ALA D 728     133.199 -10.624  30.846  1.00 17.98      D
ATOM   9144  N   ALA D 729     133.823  -9.315  32.605  1.00 24.10      D
ATOM   9145  CA  ALA D 729     135.175  -9.868  32.740  1.00 25.79      D
ATOM   9146  CB  ALA D 729     136.139  -8.792  33.225  1.00 26.49      D
ATOM   9147  C   ALA D 729     135.036 -10.980  33.770  1.00 26.20      D
ATOM   9148  O   ALA D 729     134.619 -10.736  34.900  1.00 24.79      D
ATOM   9149  N   VAL D 730     135.363 -12.199  33.351  1.00 27.91      D
ATOM   9150  CA  VAL D 730     135.224 -13.396  34.182  1.00 28.52      D
ATOM   9151  CB  VAL D 730     134.162 -14.349  33.578  1.00 25.65      D
ATOM   9152  CG1 VAL D 730     132.846 -13.619  33.401  1.00 21.69      D
ATOM   9153  CG2 VAL D 730     134.667 -14.910  32.251  1.00 23.86      D
ATOM   9154  C   VAL D 730     136.496 -14.215  34.373  1.00 30.60      D
ATOM   9155  O   VAL D 730     137.544 -13.945  33.773  1.00 29.25      D
ATOM   9156  N   GLU D 731     136.373 -15.227  35.224  1.00 34.05      D
ATOM   9157  CA  GLU D 731     137.468 -16.136  35.507  1.00 38.43      D
ATOM   9158  CB  GLU D 731     138.069 -15.875  36.877  1.00 39.08      D
ATOM   9159  CG  GLU D 731     139.163 -16.851  37.195  1.00 41.06      D
ATOM   9160  CD  GLU D 731     139.469 -16.908  38.664  1.00 44.19      D
ATOM   9161  OE1 GLU D 731     139.986 -15.898  39.204  1.00 43.94      D
ATOM   9162  OE2 GLU D 731     139.184 -17.969  39.275  1.00 45.15      D
ATOM   9163  C   GLU D 731     136.915 -17.541  35.481  1.00 39.52      D
ATOM   9164  O   GLU D 731     136.003 -17.862  36.239  1.00 38.90      D
ATOM   9165  N   LYS D 732     137.464 -18.375  34.606  1.00 42.02      D
ATOM   9166  CA  LYS D 732     137.000 -19.744  34.487  1.00 44.14      D
ATOM   9167  CB  LYS D 732     136.079 -19.864  33.279  1.00 45.79      D
ATOM   9168  CG  LYS D 732     135.263 -21.130  33.269  1.00 48.52      D
ATOM   9169  CD  LYS D 732     134.329 -21.169  32.074  1.00 48.95      D
ATOM   9170  CE  LYS D 732     133.753 -22.555  31.897  1.00 50.73      D
ATOM   9171  NZ  LYS D 732     132.777 -22.576  30.795  1.00 53.14      D
ATOM   9172  C   LYS D 732     138.155 -20.724  34.366  1.00 45.13      D
ATOM   9173  O   LYS D 732     139.012 -20.593  33.491  1.00 46.00      D
ATOM   9174  N   ASP D 733     138.179 -21.702  35.263  1.00 45.68      D
ATOM   9175  CA  ASP D 733     139.227 -22.710  35.263  1.00 45.99      D
ATOM   9176  CB  ASP D 733     139.114 -23.590  34.013  1.00 47.96      D
ATOM   9177  CG  ASP D 733     137.759 -24.322  33.917  1.00 51.97      D
```

```
ATOM   9178  OD1 ASP D 733     137.355 -24.977  34.905  1.00 55.70      D
ATOM   9179  OD2 ASP D 733     137.095 -24.256  32.855  1.00 50.55      D
ATOM   9180  C   ASP D 733     140.603 -22.066  35.311  1.00 45.97      D
ATOM   9181  O   ASP D 733     141.493 -22.456  34.565  1.00 46.45      D
ATOM   9182  N   GLY D 734     140.778 -21.075  36.182  1.00 45.60      D
ATOM   9183  CA  GLY D 734     142.072 -20.420  36.295  1.00 44.79      D
ATOM   9184  C   GLY D 734     142.438 -19.447  35.182  1.00 44.98      D
ATOM   9185  O   GLY D 734     143.607 -19.089  35.012  1.00 44.45      D
ATOM   9186  N   GLN D 735     141.453 -19.010  34.411  1.00 43.41      D
ATOM   9187  CA  GLN D 735     141.747 -18.067  33.349  1.00 42.41      D
ATOM   9188  CB  GLN D 735     141.935 -18.820  32.034  1.00 44.33      D
ATOM   9189  CG  GLN D 735     143.185 -19.679  32.036  1.00 46.62      D
ATOM   9190  CD  GLN D 735     143.303 -20.555  30.810  1.00 48.33      D
ATOM   9191  OE1 GLN D 735     143.228 -20.076  29.670  1.00 49.33      D
ATOM   9192  NE2 GLN D 735     143.495 -21.853  31.035  1.00 48.62      D
ATOM   9193  C   GLN D 735     140.647 -17.025  33.243  1.00 40.32      D
ATOM   9194  O   GLN D 735     139.504 -17.282  33.609  1.00 40.35      D
ATOM   9195  N   SER D 736     141.001 -15.841  32.765  1.00 37.70      D
ATOM   9196  CA  SER D 736     140.033 -14.770  32.630  1.00 35.67      D
ATOM   9197  CB  SER D 736     140.664 -13.454  33.051  1.00 35.55      D
ATOM   9198  OG  SER D 736     141.815 -13.209  32.262  1.00 33.28      D
ATOM   9199  C   SER D 736     139.580 -14.656  31.191  1.00 35.08      D
ATOM   9200  O   SER D 736     140.375 -14.823  30.273  1.00 35.01      D
ATOM   9201  N   PHE D 737     138.299 -14.370  30.998  1.00 35.00      D
ATOM   9202  CA  PHE D 737     137.749 -14.215  29.662  1.00 34.26      D
ATOM   9203  CB  PHE D 737     136.928 -15.436  29.259  1.00 34.41      D
ATOM   9204  CG  PHE D 737     137.736 -16.689  29.121  1.00 34.85      D
ATOM   9205  CD1 PHE D 737     138.122 -17.416  30.243  1.00 34.24      D
ATOM   9206  CD2 PHE D 737     138.120 -17.140  27.864  1.00 34.84      D
ATOM   9207  CE1 PHE D 737     138.871 -18.574  30.108  1.00 34.16      D
ATOM   9208  CE2 PHE D 737     138.868 -18.293  27.724  1.00 33.97      D
ATOM   9209  CZ  PHE D 737     139.246 -19.012  28.845  1.00 34.14      D
ATOM   9210  C   PHE D 737     136.869 -12.992  29.611  1.00 33.97      D
ATOM   9211  O   PHE D 737     136.627 -12.359  30.639  1.00 34.16      D
ATOM   9212  N   LEU D 738     136.387 -12.673  28.411  1.00 32.98      D
ATOM   9213  CA  LEU D 738     135.526 -11.514  28.199  1.00 33.21      D
ATOM   9214  CB  LEU D 738     136.222 -10.527  27.255  1.00 32.13      D
ATOM   9215  CG  LEU D 738     135.744  -9.075  27.237  1.00 32.97      D
ATOM   9216  CD1 LEU D 738     134.465  -8.962  26.461  1.00 33.24      D
ATOM   9217  CD2 LEU D 738     135.574  -8.569  28.668  1.00 33.16      D
ATOM   9218  C   LEU D 738     134.180 -11.955  27.620  1.00 33.76      D
ATOM   9219  O   LEU D 738     134.110 -12.360  26.473  1.00 36.66      D
ATOM   9220  N   GLU D 739     133.114 -11.870  28.410  1.00 33.64      D
ATOM   9221  CA  GLU D 739     131.793 -12.292  27.959  1.00 32.51      D
ATOM   9222  CB  GLU D 739     131.000 -12.884  29.121  1.00 33.25      D
ATOM   9223  CG  GLU D 739     131.529 -14.166  29.668  1.00 34.95      D
ATOM   9224  CD  GLU D 739     131.644 -15.235  28.602  1.00 38.68      D
ATOM   9225  OE1 GLU D 739     130.731 -15.323  27.733  1.00 38.32      D
ATOM   9226  OE2 GLU D 739     132.651 -15.991  28.646  1.00 39.63      D
ATOM   9227  C   GLU D 739     130.961 -11.163  27.377  1.00 32.88      D
ATOM   9228  O   GLU D 739     130.735 -10.144  28.044  1.00 33.94      D
ATOM   9229  N   ILE D 740     130.487 -11.329  26.147  1.00 31.70      D
ATOM   9230  CA  ILE D 740     129.641 -10.301  25.568  1.00 29.64      D
ATOM   9231  CB  ILE D 740     130.288  -9.670  24.299  1.00 28.27      D
```

```
ATOM   9232  CG2 ILE D 740     129.461  -8.484  23.831  1.00 27.08      D
ATOM   9233  CG1 ILE D 740     131.663  -9.093  24.620  1.00 24.97      D
ATOM   9234  CD1 ILE D 740     132.282  -8.385  23.424  1.00 24.47      D
ATOM   9235  C   ILE D 740     128.275 -10.906  25.252  1.00 29.65      D
ATOM   9236  O   ILE D 740     128.174 -11.845  24.470  1.00 30.71      D
ATOM   9237  N   LEU D 741     127.226 -10.388  25.885  1.00 30.03      D
ATOM   9238  CA  LEU D 741     125.872 -10.903  25.659  1.00 30.25      D
ATOM   9239  CB  LEU D 741     125.209 -11.213  26.994  1.00 30.19      D
ATOM   9240  CG  LEU D 741     126.016 -12.176  27.872  1.00 30.17      D
ATOM   9241  CD1 LEU D 741     125.458 -12.120  29.284  1.00 31.69      D
ATOM   9242  CD2 LEU D 741     125.969 -13.591  27.323  1.00 26.90      D
ATOM   9243  C   LEU D 741     125.012  -9.935  24.863  1.00 29.80      D
ATOM   9244  O   LEU D 741     124.939  -8.750  25.176  1.00 28.77      D
ATOM   9245  N   ASP D 742     124.354 -10.462  23.837  1.00 31.56      D
ATOM   9246  CA  ASP D 742     123.513  -9.664  22.948  1.00 32.74      D
ATOM   9247  CB  ASP D 742     123.917  -9.906  21.492  1.00 33.83      D
ATOM   9248  CG  ASP D 742     123.601  -8.730  20.592  1.00 34.30      D
ATOM   9249  OD1 ASP D 742     122.422  -8.315  20.526  1.00 33.76      D
ATOM   9250  OD2 ASP D 742     124.550  -8.223  19.952  1.00 34.48      D
ATOM   9251  C   ASP D 742     122.046 -10.021  23.110  1.00 33.39      D
ATOM   9252  O   ASP D 742     121.617 -11.102  22.713  1.00 33.45      D
ATOM   9253  N   PHE D 743     121.283  -9.097  23.685  1.00 34.50      D
ATOM   9254  CA  PHE D 743     119.858  -9.296  23.905  1.00 34.56      D
ATOM   9255  CB  PHE D 743     119.422  -8.544  25.161  1.00 32.05      D
ATOM   9256  CG  PHE D 743     119.627  -9.324  26.400  1.00 29.59      D
ATOM   9257  CD1 PHE D 743     120.893  -9.462  26.941  1.00 27.43      D
ATOM   9258  CD2 PHE D 743     118.579 -10.058  26.935  1.00 28.98      D
ATOM   9259  CE1 PHE D 743     121.116 -10.332  27.987  1.00 26.97      D
ATOM   9260  CE2 PHE D 743     118.787 -10.933  27.980  1.00 27.93      D
ATOM   9261  CZ  PHE D 743     120.059 -11.077  28.507  1.00 26.94      D
ATOM   9262  C   PHE D 743     118.973  -8.895  22.734  1.00 35.12      D
ATOM   9263  O   PHE D 743     117.746  -8.889  22.849  1.00 35.80      D
ATOM   9264  N   SER D 744     119.594  -8.592  21.600  1.00 35.35      D
ATOM   9265  CA  SER D 744     118.854  -8.176  20.416  1.00 35.76      D
ATOM   9266  CB  SER D 744     119.823  -7.612  19.381  1.00 36.40      D
ATOM   9267  OG  SER D 744     119.126  -6.857  18.417  1.00 40.54      D
ATOM   9268  C   SER D 744     118.029  -9.301  19.793  1.00 35.75      D
ATOM   9269  O   SER D 744     118.433 -10.488  19.873  1.00 36.28      D
ATOM   9270  OXT SER D 744     116.984  -8.972  19.209  1.00 34.82      D
ATOM   9271  CB  LEU E   2      57.203  -3.013  76.696  1.00 93.40      E
ATOM   9272  CG  LEU E   2      56.802  -2.909  78.154  1.00 92.64      E
ATOM   9273  CD1 LEU E   2      56.089  -4.209  78.494  1.00 92.62      E
ATOM   9274  CD2 LEU E   2      58.002  -2.716  79.063  1.00 91.70      E
ATOM   9275  C   LEU E   2      58.910  -2.837  74.950  1.00 94.06      E
ATOM   9276  O   LEU E   2      59.052  -4.056  75.064  1.00 94.80      E
ATOM   9277  N   LEU E   2      57.498  -0.813  75.549  1.00 93.79      E
ATOM   9278  CA  LEU E   2      58.180  -2.054  76.029  1.00 93.74      E
ATOM   9279  N   LEU E   3      59.349  -2.162  73.890  1.00 93.32      E
ATOM   9280  CA  LEU E   3      60.093  -2.853  72.840  1.00 91.84      E
ATOM   9281  CB  LEU E   3      60.099  -2.030  71.539  1.00 90.21      E
ATOM   9282  CG  LEU E   3      58.738  -2.011  70.818  1.00 88.51      E
ATOM   9283  CD1 LEU E   3      58.863  -1.419  69.431  1.00 86.61      E
ATOM   9284  CD2 LEU E   3      58.194  -3.426  70.729  1.00 87.78      E
ATOM   9285  C   LEU E   3      61.504  -3.132  73.355  1.00 91.93      E
```

```
ATOM   9286  O   LEU E   3      62.459  -2.428  73.011  1.00 92.22      E
ATOM   9287  N   TPO E   4      61.634  -4.171  74.204  1.00 91.56      E
ATOM   9288  CA  TPO E   4      62.536  -4.975  75.032  1.00 90.52      E
ATOM   9289  CB  TPO E   4      62.853  -4.058  76.249  1.00 89.37      E
ATOM   9290  CG2 TPO E   4      63.717  -4.740  77.314  1.00 89.39      E
ATOM   9291  OG1 TPO E   4      63.546  -2.864  75.833  1.00 86.87      E
ATOM   9292  P   TPO E   4      65.016  -2.884  75.092  1.00 83.35      E
ATOM   9293  O1P TPO E   4      64.849  -3.624  73.731  1.00 83.36      E
ATOM   9294  O2P TPO E   4      66.088  -3.641  76.006  1.00 83.80      E
ATOM   9295  O3P TPO E   4      65.359  -1.340  74.831  1.00 84.80      E
ATOM   9296  C   TPO E   4      61.804  -6.259  75.507  1.00 91.34      E
ATOM   9297  O   TPO E   4      60.467  -6.316  75.619  1.00 91.46      E
ATOM   9298  N   PRO E   5      63.256  -5.997  71.948  1.00 83.51      E
ATOM   9299  CD  PRO E   5      63.441  -4.606  71.529  1.00 83.14      E
ATOM   9300  CA  PRO E   5      63.931  -6.885  71.003  1.00 84.53      E
ATOM   9301  CB  PRO E   5      65.159  -6.089  70.575  1.00 83.61      E
ATOM   9302  CG  PRO E   5      64.831  -4.637  70.919  1.00 83.06      E
ATOM   9303  C   PRO E   5      64.316  -8.236  71.564  1.00 85.50      E
ATOM   9304  O   PRO E   5      64.916  -8.330  72.628  1.00 85.67      E
ATOM   9305  N   PRO E   6      63.969  -9.312  70.847  1.00 86.93      E
ATOM   9306  CD  PRO E   6      63.085  -9.303  69.669  1.00 87.22      E
ATOM   9307  CA  PRO E   6      64.267 -10.690  71.255  1.00 88.33      E
ATOM   9308  CB  PRO E   6      63.629 -11.522  70.149  1.00 87.80      E
ATOM   9309  CG  PRO E   6      62.478 -10.688  69.722  1.00 87.62      E
ATOM   9310  C   PRO E   6      65.765 -10.988  71.384  1.00 89.85      E
ATOM   9311  O   PRO E   6      66.575 -10.544  70.557  1.00 90.61      E
ATOM   9312  N   GLN E   7      66.126 -11.745  72.421  1.00 90.83      E
ATOM   9313  CA  GLN E   7      67.515 -12.125  72.626  1.00 91.45      E
ATOM   9314  CB  GLN E   7      68.006 -11.682  73.992  1.00 91.16      E
ATOM   9315  CG  GLN E   7      68.555 -10.282  73.957  1.00 91.12      E
ATOM   9316  CD  GLN E   7      69.842 -10.165  74.739  1.00 91.14      E
ATOM   9317  OE1 GLN E   7      69.851 -10.287  75.975  1.00 92.25      E
ATOM   9318  NE2 GLN E   7      70.950  -9.958  74.025  1.00 89.30      E
ATOM   9319  C   GLN E   7      67.666 -13.631  72.485  1.00 91.90      E
ATOM   9320  O   GLN E   7      67.429 -14.383  73.431  1.00 92.11      E
ATOM   9321  N   SER E   8      68.051 -14.055  71.282  1.00 92.25      E
ATOM   9322  CA  SER E   8      68.235 -15.467  70.933  1.00 92.14      E
ATOM   9323  CB  SER E   8      67.113 -15.896  69.981  1.00 92.25      E
ATOM   9324  OG  SER E   8      66.978 -17.305  69.938  1.00 92.67      E
ATOM   9325  C   SER E   8      69.603 -15.640  70.258  1.00 92.02      E
ATOM   9326  O   SER E   8      70.638 -15.398  70.879  1.00 91.94      E
ATOM   9327  N   GLY E   9      69.602 -16.057  68.994  1.00 91.78      E
ATOM   9328  CA  GLY E   9      70.854 -16.235  68.277  1.00 91.39      E
ATOM   9329  C   GLY E   9      70.848 -15.537  66.928  1.00 91.23      E
ATOM   9330  O   GLY E   9      69.743 -15.212  66.445  1.00 90.99      E
ATOM   9331  OXT GLY E   9      71.939 -15.322  66.346  1.00 90.21      E
ATOM   9332  CB  LEU F   2     137.489  -5.702  48.818  1.00 79.71      F
ATOM   9333  CG  LEU F   2     138.842  -5.743  49.546  1.00 80.18      F
ATOM   9334  CD1 LEU F   2     139.667  -4.549  49.099  1.00 79.66      F
ATOM   9335  CD2 LEU F   2     138.661  -5.730  51.075  1.00 78.72      F
ATOM   9336  C   LEU F   2     138.487  -6.493  46.630  1.00 78.95      F
ATOM   9337  O   LEU F   2     138.336  -7.720  46.632  1.00 77.64      F
ATOM   9338  N   LEU F   2     136.056  -5.715  46.790  1.00 79.28      F
ATOM   9339  CA  LEU F   2     137.454  -5.545  47.286  1.00 79.36      F
```

```
ATOM   9340  N   LEU F   3     139.520  -5.871  46.060  1.00 78.25      F
ATOM   9341  CA  LEU F   3     140.670  -6.502  45.403  1.00 76.54      F
ATOM   9342  CB  LEU F   3     140.433  -6.740  43.915  1.00 77.32      F
ATOM   9343  CG  LEU F   3     139.459  -7.802  43.429  1.00 78.88      F
ATOM   9344  CD1 LEU F   3     138.100  -7.190  43.081  1.00 80.14      F
ATOM   9345  CD2 LEU F   3     140.065  -8.449  42.204  1.00 78.71      F
ATOM   9346  C   LEU F   3     141.723  -5.415  45.530  1.00 75.20      F
ATOM   9347  O   LEU F   3     141.444  -4.264  45.195  1.00 75.82      F
ATOM   9348  N   TPO F   4     142.936  -5.746  46.012  1.00 72.87      F
ATOM   9349  CA  TPO F   4     144.008  -4.734  46.163  1.00 70.82      F
ATOM   9350  CB  TPO F   4     144.161  -4.534  47.709  1.00 68.53      F
ATOM   9351  CG2 TPO F   4     145.393  -3.748  48.146  1.00 70.46      F
ATOM   9352  OG1 TPO F   4     142.965  -3.903  48.203  1.00 65.51      F
ATOM   9353  P   TPO F   4     142.778  -2.260  48.081  1.00 60.19      F
ATOM   9354  O1P TPO F   4     142.871  -1.889  46.565  1.00 64.16      F
ATOM   9355  O2P TPO F   4     143.905  -1.501  48.889  1.00 62.63      F
ATOM   9356  O3P TPO F   4     141.319  -1.975  48.672  1.00 64.49      F
ATOM   9357  C   TPO F   4     145.311  -5.244  45.579  1.00 70.94      F
ATOM   9358  O   TPO F   4     145.629  -6.541  45.562  1.00 71.31      F
ATOM   9359  N   PRO F   5     146.116  -4.278  45.081  1.00 71.04      F
ATOM   9360  CD  PRO F   5     145.651  -2.886  44.895  1.00 69.22      F
ATOM   9361  CA  PRO F   5     147.434  -4.439  44.468  1.00 71.37      F
ATOM   9362  CB  PRO F   5     147.722  -3.051  43.898  1.00 70.57      F
ATOM   9363  CG  PRO F   5     146.379  -2.473  43.673  1.00 68.58      F
ATOM   9364  C   PRO F   5     148.447  -4.823  45.533  1.00 72.63      F
ATOM   9365  O   PRO F   5     148.273  -4.524  46.709  1.00 72.26      F
ATOM   9366  N   PRO F   6     149.531  -5.484  45.133  1.00 74.58      F
ATOM   9367  CD  PRO F   6     149.883  -5.888  43.760  1.00 74.65      F
ATOM   9368  CA  PRO F   6     150.563  -5.898  46.087  1.00 76.44      F
ATOM   9369  CB  PRO F   6     151.636  -6.499  45.180  1.00 76.17      F
ATOM   9370  CG  PRO F   6     150.843  -7.015  44.005  1.00 75.36      F
ATOM   9371  C   PRO F   6     151.108  -4.721  46.907  1.00 78.12      F
ATOM   9372  O   PRO F   6     151.745  -3.827  46.351  1.00 78.87      F
ATOM   9373  N   GLN F   7     150.858  -4.699  48.213  1.00 79.62      F
ATOM   9374  CA  GLN F   7     151.397  -3.605  49.020  1.00 81.37      F
ATOM   9375  CB  GLN F   7     150.607  -3.435  50.333  1.00 81.68      F
ATOM   9376  CG  GLN F   7     151.014  -2.213  51.171  1.00 82.68      F
ATOM   9377  CD  GLN F   7     150.936  -0.896  50.397  1.00 83.36      F
ATOM   9378  OE1 GLN F   7     151.562  -0.740  49.343  1.00 84.22      F
ATOM   9379  NE2 GLN F   7     150.175   0.061  50.927  1.00 82.82      F
ATOM   9380  C   GLN F   7     152.866  -3.939  49.299  1.00 82.45      F
ATOM   9381  O   GLN F   7     153.186  -4.607  50.282  1.00 82.78      F
ATOM   9382  N   SER F   8     153.745  -3.472  48.411  1.00 83.82      F
ATOM   9383  CA  SER F   8     155.196  -3.704  48.479  1.00 85.47      F
ATOM   9384  CB  SER F   8     155.937  -2.583  47.732  1.00 84.24      F
ATOM   9385  OG  SER F   8     155.277  -2.236  46.527  1.00 83.28      F
ATOM   9386  C   SER F   8     155.813  -3.857  49.887  1.00 86.86      F
ATOM   9387  O   SER F   8     156.285  -2.881  50.482  1.00 87.36      F
ATOM   9388  N   GLY F   9     155.830  -5.093  50.390  1.00 87.52      F
ATOM   9389  CA  GLY F   9     156.387  -5.374  51.708  1.00 87.82      F
ATOM   9390  C   GLY F   9     155.445  -6.117  52.646  1.00 87.94      F
ATOM   9391  O   GLY F   9     154.243  -6.240  52.319  1.00 88.07      F
ATOM   9392  OXT GLY F   9     155.901  -6.573  53.717  1.00 87.76      F
END
```

Table 7.
Oligonucleotides used in Example 2

MTO#	Oligo name	Sequence
MTO 1146	LP6DelA-FWD	gccttcgcgaactgatgtacactttgcagggtcatacagc
MTO 1147	LP6DelA-REV	gccttggccattttctagatcccaaattctaatagtggtatccatac
MTO 1254	CDC4-BNSH-F	gtaggatccatatgggcgccgcaagctttcccttagctgagtttcc
MTO 1367	V384N-C	catatgacgagtaatattacgtgcttgc
MTO 1368	V384N3	caagcacgtaatattactcgtcatatg
MTO 1369	K402A-C	ggggctgatgacgcaatgatcagag
MTO 1370	K402A-N	ctctgatcattgcgtcatcagcccc
MTO 1371	W426A 5'	gatggtggggttgcggcgctgaagtatgcccatg
MTO 1372	DN426A	catgggcatacttcagcgccgcaaccccaccatc
MTO 1373	R443D-C	ggttctacagacgacacggtccgagtttggg
MTO 1374	R443D	tatcccaaactcggaccgtgtcgtcgtctgtagaaccg
MTO 1375	Y548F	cagtgtattatcaaagcttccactaacgac
MTO 1376	Y548F-C	gtcgttagtggaagctttgataatacactg
MTO 1377	Y574F-N	gtagattgtcgaaaatattcgatccgtatg
MTO 1378	Y574F-C	catacggatcgaatattttcgacaatctac
MTO 1379	W717N Hpa	ttgcccttaaagttaaccgagttaatctgatcag
MTO 1380	W717N-C	ctgatcagattaactcggttaactttaagggcaa
MTO 1381	2Flex359 5'	tcttttctggagcccgggccaattttaaaaaattggtac
MTO 1382	2Flex359 3'	gtaccaatttttttaaaattggcccgggctccagaaaaga
MTO 1383	H5 Dest 5'	ggttttaattctctcggcccgggaccctcccaaaaataccaaaactc
MTO 1384	H5 Dest 3'	gagttttgggtatttttgggagggtcccgggccgagagaattaaaacc
MTO 1385	H5 del 5'	gtgagcccaaagggtccaaagctttcacaacaagatcgc
MTO 1386	H5 del 3'	gcgatcttgttgtgaaagctttggacccttgggctcac
MTO 1387	H5+ Dest 5'	gtggaaaaaacttctgatattcattttaaaaaattggtacaatcc
MTO 1388	H5+ Dest 3'	ggattgtaccaatttttttaaaatgaatatcagaagtttttttccac
MTO 1389	Ala1-3	ccaatttttttaaaatgaatgcaatattctccagaaaag
MTO 1390	Ala2-3	ccaatttttttaaaatgaatgctgcaatattctccagaaaag
MTO 1391	Ala3-3	ccaatttttttaaaatgaaagcggctgcaatattctccagaaaag
MTO 1392	Ala4-3	ccaatttttttaaaatgaaggctgcagctgcaatattctccagaaaag
MTO 1393	Ala8 5'	gccgcgcgcgctaaagctgcagcgttcattttaaaaaattggtacaatcc
MTO 1394	Ala8 3'	cgctgcagctttagcgcgcgcggctatattctccagaaaagataatc
MTO 1395	Ala12 5'	gccgcgcgcgctaaagctgcagcgcgcgcgaaagccttcattttaaaaaattggtacaatcc
MTO 1396	Al12 3'	ggctttcgcgcgcgctgcagctttagcgcgcgcggctatattctccagaaaagataatc

Table 8.
Plasmids used in Example 2

Plasmid	Relevant Characteristic	Source
pMT 3169	pProEx Hta-CDC4 LP6DelA GST-Skp1	This study
pMT 3055	pProEx Hta-CDC4 263-744 GST-Skp1	Nash et. al.
pMT 3000	pProEx Hta-CDC4 1-744 GST-Skp1	This study
pMT 3217	pRS 314 CDC4-BNSH/Eco	This study
pMT 3001	pMT 3055 V384N	This study
pMT 3002	pMT 3055 K402A	This study
pMT 3385	pMT 3055 W426A	This study
pMT 3058	pMT 3055 R443A	Nash et. al
pMT 3003	pMT 3055 R443D	This study
pMT 3059	pMT 3055 R467A	Nash et. al
pMT 3060	pMT 3055 R485A	Nash et. al
pMT 3061	pMT 3055 R534A	Nash et. al
pMT 3004	pMT 3055 Y548F	This study
pMT 3005	pMT 3055 Y574F	This study
pMT 3006	pMT 3055 W717N	This study
pMT 3007	pMT 3055 V384N+W717N	This study
pMT 3008	pMT 3055 K402+R443D	This study
pMT 3010	pMT 3000 R443D	This study
pMT 3011	pMT 3000 R443A	This study
pMT 3012	pMT 3000 W717N	This study
pMT 3013	pMT 3000 K402A+R443D	This study
pMT 3014	pMT 3000 V384N+W717N	This study
pMT 3015	pMT 3217 V384N	This study
pMT 3016	pMT 3217 K402A	This study
pMT 3386	pMT 3217 W426A	This study
pMT 3017	pMT 3217 R443D	This study
pMT 3058	PRS 314-CDC4 R443A	Nash et. al.
pMT 3018	pMT 3217 Y548F	This study
pMT 3068	PRS 314-CDC4 R572A	Nash et. al
pMT 3019	pMT 3217 Y574F	This study
pMT 3020	pMT 3217 W717N	This study
pMT 3021	pMT 3217 V384N+W717N	This study
pMT 3022	pMT 3217 K402A+R443D	This study
pMT 3024	pMT 3000 Helix 5 Δ 330-443	This study
pMT 3025	pMT 3000 Helix 5 breaker	This study
pMT 3026	pMT 3000 Helix 5 Δ 321-360	This study
pMT 3027	pMT 3000 Helix 6 breaker	This study
pMT 3028	pMT 3000 Ala1 insert	This study
pMT 3029	pMT 3000 Ala2 insert	This study
pMT 3030	pMT 3000 Ala3 insert	This study
pMT 3031	pMT 3000 Ala4 insert	This study
pMT 3032	pMT 3000 Ala8 insert	This study
pMT 3033	pMT 3000 Ala12 insert	This study
pMT 3034	pMT 3217 Helix 5 Δ 330-443	This study
pMT 3035	pMT 3217 Helix 5 breaker	This study
pMT 3036	pMT 3217 Helix 5 Δ 321-360	This study

Plasmid	Relevant Characteristic	Source
pMT 3037	pMT 3217 Helix 6 breaker	This study
pMT 3038	pMT 3217 Ala1 insert	This study
pMT 3039	pMT 3217 Ala2 insert	This study
pMT 3040	pMT 3217 Ala3 insert	This study
pMT 3041	pMT 3217 Ala4 insert	This study
pMT 3042	pMT 3217 Ala8 insert	This study
pMT 3043	pMT 3217 Ala12 insert	This study
pMT 1571	Pet16b-Sic1	Previous study
MDM 152	pGAL1 SIC1 LEU2 CEN ARS	M. Mendenhall
MDM202	pGAL1 SIC1^{T33V} LEU2 CEN ARS	M. Mendenhall

List of References

1. Amati, B., and Vlach, J. (1999). Kip1 meets SKP2: new links in cell-cycle control [news], Nat Cell Biol *1*, E91-3.
2. Bai, C., Sen, P., Hofmann, K., Ma, L., Goebl, M., Harper, J. W., and Elledge, S. J. (1996). SKP1 connects cell cycle regulators to the ubiquitin proteolysis machinery through a novel motif, the F-box, Cell *86*, 263-74.
3. Brunger, A. T., Adams, P. D., Clore, G. M., Gros, P., Grosse-Kuntsleve, Jiang, R. W., Kuszewski, J., Nilges, M., Pannu, N. S., Read, R. J., and al., e. (1998). Crystallography and NMR system: a new software suite for macromolecular structure determination. Acta Cryst. *D54*, 905-921.
4. Carson, M. (1991). Ribbons 2.0. J. Appl. Crystallgr. *24*, 958-961.
5. Chi, Y., Huddleston, M. J., Zhang, X., Young, R. A., Annan, R. S., Carr, S. A., and Deshaies, R. J. (2001). Negative regulation of Gcn4 and Msn2 transcription factors by Srb10 cyclin-dependent kinase. Genes. Dev. *15*, 1078-1092.
6. Cohen, P. (2000). The regulation of protein function by multisite phosphorylation: a 25 year update. Trends Biochem. Sci. *25*, 596-601.
7. de La Fortelle, E., and Bricogne, G. (1997). Maximum-likelihood heavy-atom parameter refinement for multiple isomorphous replacement and multiwavelength anomalous diffraction methods. Methods Enzymol. *276*, 472-494.
8. Deshaies, R. J. (1999). SCF and Cullin/Ring H2-based ubiquitin ligases, Annu Rev Cell Dev Biol *15*, 435-67.
9. Deshaies, R. J., and Ferrell, J. E., Jr. (2001). Multisite phosphorylation and the countdown to S phase, Cell *107*, 819-22.
10. Drury, L. S., Perkins, G., and Diffley, J. F. (1997). The Cdc4/34/53 pathway targets Cdc6p for proteolysis in budding yeast, Embo J *16*, 5966-76.
11. Eck, M. J., Pluskey, S., Trub, T., Harrison, S. C., and Shoelson, S. E. (1996). Spatial constraints on the recognition of phosphoproteins by the tandem SH2 domains of the phosphatase SH-PTP2, Nature *379*, 277-80.
12. Endicott, J. A., Noble, M. E., and Tucker, J. A. (1999). Cyclin-dependent kinases: inhibition and substrate recognition. Curr. Opin. Struct. Biol. *9*, 738-744.
13. Feldman, R. M., Correll, C. C., Kaplan, K. B., and Deshaies, R. J. (1997). A complex of Cdc4p, Skp1p, and Cdc53p/cullin catalyzes ubiquitination of the phosphorylated CDK inhibitor Sic1p, Cell *91*, 221-30.
14. Ferrell, J. E. (1996). Tripping the switch fantastic: how a protein kinase cascade can convert graded inputs into switch-like outputs, Trends Biochem Sci *21*, 460-466.
15. Fulop, V., and Jones, D. T. (1999). Beta propellers: structural rigidity and functional diversity., Curr Opin Struct Biol *9*, 715-721.

16. Gstaiger, M., Jordan, R., Lim, M., Catzavelos, C., Mestan, J., Slingerland, J., and Krek, W. (2001). Skp2 is oncogenic and overexpressed in human cancers, Proc Natl Acad Sci U S A *98*, 5043-8.

17. Gupta-Rossi, N., Le Bail, O., Gonen, H., Brou, C., Logeat, F., Six, E., Ciechanover, A., and Israel, A. (2002). Functional interaction between SEL-10, an F-box protein, and the nuclear form of activated Notch1 receptor, J Biol Chem *276*, 34371-34378.

18. Hamilton, K. S., Ellison, M. J., Barber, K. R., Williams, R. S., Huzil, J. T., McKenna, S., Ptak, C., Glover, M., and Shaw, G. S. (2001). Structure of a conjugating enzyme-ubiquitin thiolester intermediate reveals a novel role for the ubiquitin tail. Structure *9*, 897-904.

19. Harper, J. W. (2001). Protein destruction: adapting roles for Cks proteins. Curr Biol *11*, R431-435.

20. Harper, J. W. (2002). A phosphorylation-driven ubiquitination switch for cell-cycle control, Trends Cell Biol *12*, 104-7.

21. Hershko, A., and Ciechanover, A. (1998). The ubiquitin system, Annu Rev Biochem *67*, 425-79.

22. Hershko, D., Bornstein, G., Ben-Izhak, O., Carrano, A., Pagano, M., Krausz, M. M., and Hershko, A. (2001). Inverse relation between levels of p27(Kip1) and of its ubiquitin ligase subunit Skp2 in colorectal carcinomas, Cancer *91*, 1745-51.

23. Hsiung, Y. G., Chang, H. C., Pellequer, J. L., La Valle, R., Lanker, S., and Wittenberg, C. (2001). F-box protein Grr1 interacts with phosphorylated targets via the cationic surface of its leucine-rich repeat, Mol Cell Biol *21*, 2506-20.

24. Huang, L., Kinnucan, E., Wang, G., Beaudenon, S., Howley, P. M., Huibregtse, J. M., and Pavletich, N. P. (1999). Structure of an E6AP-UbcH7 complex: insights into ubiquitination by the E2-E3 enzyme cascade, Science *286*, 1321-6.

25. Hubbard, E. J., Wu, G., Kitajewski, J., and Greenwald, I. (1997). sel-10, a negative regulator of lin-12 activity in Caenorhabditis elegans, encodes a member of the CDC4 family of proteins, Genes Dev *11*, 3182-93.

26. Jones, T. A., Zou, J. Y., Cowan, S. W., and Kjeldgaard, M. (1991). Improved methods for binding protein models in electron density maps and the localization of errors in these models. Acta Cryst. *A47*, 110-119.

27. Kaelin, W. G., Jr. (2002). Molecular basis of the VHL hereditary cancer syndrome. Nat. Rev. Cancer *2*, 673-682.

28. Keyomarsi, K., Tucker, S. L., Buchholz, T. A., Callister, M., Ding, Y., Hortobagyi, G. N., Bedrosian, I., Knickerbocker, C., Toyofuku, W., Lowe, M., *et al.* (2002). Cyclin E and survival in patients with breast cancer. N. Engl. J. Med. *347*, 1566-1575.

29. Koepp, D. M., Harper, J. W., and Elledge, S. J. (1999). How the cyclin became a cyclin: regulated proteolysis in the cell cycle, Cell *97*, 431-4.

30. Koepp, D. M., Schaefer, L. K., Ye, X., Keyomarsi, K., Chu, C., Harper, J. W., and Elledge, S. J. (2001). Phosphorylation-dependent ubiquitination of cyclin E by the SCFFbw7 ubiquitin ligase, Science *294*, 173-7.

31. Kominami, K., Ochotorena, I., and Toda, T. (1998). Two F-box/WD-repeat proteins Pop1 and Pop2 form hetero- and homo- complexes together with cullin-1 in the fission yeast SCF (Skp1-Cullin- 1-F-box) ubiquitin ligase, Genes Cells *3*, 721-35.

32. Lai, E. C. (2002). Protein degradation: four E3s for the notch pathway. Curr. Biol. *12*, R74-78.

33. Lanker, S., Valdivieso, M. H., and Wittenberg, C. (1996). Rapid degradation of the G1 cyclin Cln2 induced by CDK-dependent phosphorylation, Science *271*, 1597-601.

34. Lai, E. C. (2002). Protein degradation: four E3s for the notch pathway. Curr. Biol. *12*, R74-78.

35. Lengronne, A., and Schwob, E. (2002). The yeast CDK inhibitor Sic1 prevents genomic instability by promoting replication origin licensing in late G1. Mol. Cell. *9*, 1067-1078.

36. Mammen, M., Choi, S.-K., and Whitesides, G. M. (1998). Polyvalent interactions in biological systems: implications for design and use of multivalent ligands and inhibitors. Angew. Chem. *37*, 2754-2794.

37. Maniatis, T. (1999). A ubiquitin ligase complex essential for the NF-kappaB, Wnt/Wingless, and hedgehog signaling pathways, Genes Dev *13*, 505-510.

38. Margottin, F., Bour, S. P., Durand, H., Selig, L., Benichou, S., Richard, V., Thomas, D., Strebel, K., and Benarous, R. (1998). A novel human WD protein, h-beta TrCp, that interacts with HIV-1 Vpu connects CD4 to the ER degradation pathway through an F-box motif, Mol Cell *1*, 565-74.

39. Meimoun, A., Holtzman, T., Weissman, Z., McBride, H. J., Stillman, D. J., Fink, G. R., and Kornitzer, D. (2000). Degradation of the transcription factor Gcn4 requires the kinase Pho85 and the SCF^{CDC4} ubiquitin-ligase complex. Mol. Biol. Cell. *11*, 915-927.

40. Miller, R., Gallo, S. M., Khalak, H. G., and Weeks, C. M. (1994). SnB: crystal structure determination via Shake-and-Bake. J. Appl. Crystallgr. *27*, 613-621.

41. Moberg, K. H., Bell, D. W., Wahrer, D. C., Haber, D. A., and Hariharan, I. K. (2001). Archipelago regulates Cyclin E levels in Drosophila and is mutated in human cancer cell lines, Nature *413*, 311-6.

42. Nash, P., Tang, X., Orlicky, S., Chen, Q., Gertler, F. B., Mendenhall, M. D., Sicheri, F., Pawson, T., and Tyers, M. (2001). Multisite phosphorylation of a CDK inhibitor sets a threshold for the onset of DNA replication, Nature *414*, 514-21.

43. Nicholls, A., Sharp, K. A., and Honig, B. (1991). Protein folding and association: insights from the interfacial and thermodynamic properties of hydrocarbons. Proteins Struct. Funct. Genet. *11*, 281-296.

44. Nugroho, T. T., and Mendenhall, M. D. (1994). An inhibitor of yeast cyclin-dependent protein kinase plays an important role in ensuring the genomic integrity of daughter cells, Mol Cell Biol *14*, 3320-3328.

45. Otwinowski, Z., and Minor, W. (1997). Processing of X-ray diffraction data collected in oscillation mode. Methods Enzymol. *276*, 307-326.

46. Patton, E. E., Willems, A. R., and Tyers, M. (1998). Combinatorial control in ubiquitin-dependent proteolysis: don't Skp the F-box hypothesis, Trends Genet *14*, 236-43.

47. Pawson, T., and Nash, P. (2000). Protein-protein interactions define specificity in signal transduction., Genes Dev *14*, 1027-47.

48. Pickart, C. M. (2001). Mechanisms underlying ubiquitination, Annu Rev Biochem *70*, 503-33.

49. Sakamoto, K. M., Kim, K. B., Kumagai, A., Mercurio, F., Crews, C. M., and Deshaies, R. J. (2001). Protacs: chimeric molecules that target proteins to the Skp1-Cullin-F box complex for ubiquitination and degradation, Proc Natl Acad Sci U S A *98*, 8554-9.

50. Schneider, B. L., Yang, Q. H., and Futcher, A. B. (1996). Linkage of replication to start by the Cdk inhibitor Sic1, Science *272*, 560-2.

51. Schulman, B. A., Carrano, A. C., Jeffrey, P. D., Bowen, Z., Kinnucan, E. R., Finnin, M. S., Elledge, S. J., Harper, J. W., Pagano, M., and Pavletich, N. P. (2000). Insights into SCF ubiquitin ligases from the structure of the Skp1-Skp2 complex, Nature *408*, 381-6.

52. Schwob, E., Bohm, T., Mendenhall, M. D., and Nasmyth, K. (1994). The B-type cyclin kinase inhibitor $p40^{SIC1}$ controls the G1 to S transition in *S. cerevisiae*, Cell *79*, 233-44.

53. Selkoe, D. J. (2001). Presenilin, Notch, and the genesis and treatment of Alzheimer's disease, Proc Natl Acad Sci U S A *98*, 11039-41.

54. Signoretti, S., Di Marcotullio, L., Richardson, A., Ramaswamy, S., Isaac, B., Rue, M., Monti, F., Loda, M., and Pagano, M. (2002). Oncogenic role of the ubiquitin ligase subunit Skp2 in human breast cancer, J Clin Invest *110*, 633-41.

55. Skowyra, D., Craig, K. L., Tyers, M., Elledge, S. J., and Harper, J. W. (1997). F-box proteins are receptors that recruit phosphorylated substrates to the SCF ubiquitin-ligase complex, Cell *91*, 209-19.

56. Sprague, E. R., Redd, M. J., Johnson, A. D., and Wolberger, C. (2000). Structure of the C-terminal domain of Tup1, a corepressor of transcription in yeast, Embo J *19*, 3016-27.

57. Spruck, C. H., Strohmaier, H., Sangfelt, O., Muller, H. M., Hubalek, M., Muller-Holzner, E., Marth, C., Widschwendter, M., and Reed, S. I. (2002). hCDC4 gene mutations in endometrial cancer, Cancer Res *62*, 4535-9.

58. Spruck, C. H., Won, K. A., and Reed, S. I. (1999). Deregulated cyclin E induces chromosome instability, Nature *401*, 297-300.

59. Strohmaier, H., Spruck, C. H., Kaiser, P., Won, K. A., Sangfelt, O., and Reed, S. I. (2001). Human F-box protein hCdc4 targets cyclin E for proteolysis and is mutated in a breast cancer cell line, Nature *413*, 316-22.

60. Suzuki, H., Chiba, T., Suzuki, T., Fujita, T., Ikenoue, T., Omata, M., Furuichi, K., Shikama, H., and Tanaka, K. (2000). Homodimer of two F-box proteins betaTrCP1 or betaTrCP2 binds to IkappaBalpha for signal-dependent ubiquitination, J Biol Chem *275*, 2877-84.

61. ter Haar, E., Harrison, S. C., and Kirchhausen, T. (2000). Peptide-in-groove interactions link target proteins to the beta-propeller of clathrin., Proc Natl Acad Sci U S A *97*, 1096-100.

62. Tong, A. H., Evangelista, M., Parsons, A. B., Xu, H., Bader, G. D., Page, N., Robinson, M., Raghibizadeh, S., Hogue, C. W., Bussey, H., *et al.* (2001). Systematic genetic analysis with ordered arrays of yeast deletion mutants, Science *294*, 2364-8.

63. Tyers, M., and Jorgensen, P. (2000). Proteolysis and the cell cycle: with this RING I do thee destroy, Curr Opin Genet Dev *10*, 54-64.

64. Varshavsky, A. (1991). Naming a targeting signal, Cell *64*, 13-5.

65. Verdecia, M. A., Bowman, M. E., Lu, K. P., Hunter, T., and Noel, J. P. (2000). Structural basis for phosphoserine-proline recognition by group IV WW domains. Nat. Struct. Biol. *7*, 639-643.

66. Verma, R., Annan, R. S., Huddleston, M. J., Carr, S. A., Reynard, G., and Deshaies, R. J. (1997). Phosphorylation of Sic1p by G1 Cdk required for its degradation and entry into S phase, Science *278*, 455-460.

67. Wall, M. A., Coleman, D. E., Lee, E. I.-L., J.A.,, Posner, B. A., Gilman, A. G., and Sprang, S. R. (1995). The structure of the G protein heterotrimer Gi alpha 1 beta 1 gamma 2, Cell *83*, 1047-58.

68. Wolf, D. A., McKeon, F., and Jackson, P. K. (1999). F-box/WD-repeat proteins Pop1p and Sud1p/Pop2p form complexes that bind and direct the proteolysis of Cdc18p. Curr. Biol. *9*, 373-376.

69. Wu, G., Hubbard, E. J., Kitajewski, J. K., and Greenwald, I. (1998). Evidence for functional and physical association between Caenorhabditis elegans SEL-10, a Cdc4p-related protein, and SEL-12 presenilin., Proc Natl Acad Sci USA *95*, 15787-15891.

70. Wu, G., Lyapina, S., Das, I., Li, J., Gurney, M., Pauley, A., Chui, I., Deshaies, R. J., and Kitajewski, J. (2001). SEL-10 is an inhibitor of notch signaling that targets notch for ubiquitin-mediated protein degradation, Mol Cell Biol *21*, 7403-15.

71. Yaffe, M. B., and Elia, A. E. (2001). Phosphoserine/threonine-binding domains, Curr Opin Cell Biol *13*, 131-8.

72. Yaffe, M. B., Rittinger, K., Volinia, S., Caron, P. R., Aitken, A., Leffers, H., Gamblin, S. J., Smerdon, S. J., and Cantley, L. C. (1997). The structural basis for 14-3-3:phosphopeptide binding specificity, Cell *91*, 961-71.

73. Zachariae, W., and Nasmyth, K. (1999). Whose end is destruction: cell division and the anaphase-promoting complex, Genes Dev *13*, 2039-58.

74. Zheng, N., Schulman, B. A., Song, L., Miller, J. J., Jeffrey, P. D., Wang, P., Chu, C., Koepp, D. M., Elledge, S. J., Pagano, M., *et al.* (2002). Structure of the Cul1-Rbx1-Skp1-F boxSkp2 SCF ubiquitin ligase complex, Nature *416*, 703-9.

75. Zheng, N., Wang, P., Jeffrey, P. D., and Pavletich, N. P. (2000). Structure of a c-Cbl-UbcH7 complex: RING domain function in ubiquitin- protein ligases, Cell *102*, 533-9.